Shuvendu K. Lahiri
Chao Wang (Eds.)

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Los Angeles, CA, USA, July 21–24, 2020
Proceedings, Part II

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Preface

It was our privilege to serve as the program chairs for CAV 2020, the 32nd International Conference on Computer-Aided Verification. CAV 2020 was held as a virtual conference during July 21–24, 2020. The tutorial day was on July 20, 2020, and the pre-conference workshops were held during July 19–20, 2020. Due to the coronavirus disease (COVID-19) outbreak, all events took place online.

CAV is an annual conference dedicated to the advancement of the theory and practice of computer-aided formal analysis methods for hardware and software systems. The primary focus of CAV is to extend the frontiers of verification techniques by expanding to new domains such as security, quantum computing, and machine learning. This puts CAV at the cutting edge of formal methods research, and this year's program is a reflection of this commitment.

CAV 2020 received a very high number of submissions (240). We accepted 18 tool papers, 4 case studies, and 43 regular papers, which amounts to an acceptance rate of roughly 27%. The accepted papers cover a wide spectrum of topics, from theoretical results to applications of formal methods. These papers apply or extend formal methods to a wide range of domains such as concurrency, machine learning, and industrially deployed systems. The program featured invited talks by David Dill (Calibra) and Pushmeet Kohli (Google DeepMind) as well as invited tutorials by Tevfik Bultan (University of California, Santa Barbara) and Sriram Sankaranarayanan (University of Colorado at Boulder). Furthermore, we continued the tradition of Logic Lounge, a series of discussions on computer science topics targeting a general audience.

In addition to the main conference, CAV 2020 hosted the following workshops: Numerical Software Verification (NSV), Verified Software: Theories, Tools, and Experiments (VSTTE), Verification of Neural Networks (VNN), Democratizing Software Verification, Synthesis (SYNT), Program Equivalence and Relational Reasoning (PERR), Formal Methods for ML-Enabled Autonomous Systems (FoMLAS), Formal Methods for Blockchains (FMBC), and Verification Mentoring Workshop (VMW).

Organizing a flagship conference like CAV requires a great deal of effort from the community. The Program Committee (PC) for CAV 2020 consisted of 85 members – a committee of this size ensures that each member has to review a reasonable number of papers in the allotted time. In all, the committee members wrote over 960 reviews while investing significant effort to maintain and ensure the high quality of the conference program. We are grateful to the CAV 2020 PC for their outstanding efforts in evaluating the submissions and making sure that each paper got a fair chance. Like last year's CAV, we made the artifact evaluation mandatory for tool paper submissions and optional but encouraged for the rest of the accepted papers. The Artifact Evaluation Committee consisted of 40 reviewers who put in significant effort to evaluate each artifact. The goal of this process was to provide constructive feedback to tool developers and help make the research published in CAV more reproducible. The Artifact

Evaluation Committee was generally quite impressed by the quality of the artifacts, and, in fact, all accepted tools passed the artifact evaluation. Among the accepted regular papers, 67% of the authors submitted an artifact, and 76% of these artifacts passed the evaluation. We are also very grateful to the Artifact Evaluation Committee for their hard work and dedication in evaluating the submitted artifacts. The evaluation and selection process involved thorough online PC discussions using the EasyChair conference management system, resulting in more than 2,000 comments.

CAV 2020 would not have been possible without the tremendous help we received from several individuals, and we would like to thank everyone who helped make CAV 2020 a success. First, we would like to thank Xinyu Wang and He Zhu for chairing the Artifact Evaluation Committee and Jyotirmoy Deshmukh for local arrangements. We also thank Zvonimir Rakamaric for chairing the workshop organization, Clark Barrett for managing sponsorship, Thomas Wies for arranging student fellowships, and Yakir Vizel for handling publicity. We also thank Roopsha Samanta for chairing the Mentoring Committee. Last but not least, we would like to thank members of the CAV Steering Committee (Kenneth McMillan, Aarti Gupta, Orna Grumberg, and Daniel Kroening) for helping us with several important aspects of organizing CAV 2020.

We hope that you will find the proceedings of CAV 2020 scientifically interesting and thought-provoking!

June 2020

Shuvendu K. Lahiri
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Model Checking

Automata Tutor v3

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Abstract. Computer science class enrollments have rapidly risen in the past decade. With current class sizes, standard approaches to grading and providing personalized feedback are no longer possible and new techniques become both feasible and necessary. In this paper, we present the third version of Automata Tutor, a tool for helping teachers and students in large courses on automata and formal languages. The second version of Automata Tutor supported automatic grading and feedback for finite-automata constructions and has already been used by thousands of users in dozens of countries. This new version of Automata Tutor supports automated grading and feedback generation for a greatly extended variety of new problems, including problems that ask students to create regular expressions, context-free grammars, pushdown automata and Turing machines corresponding to a given description, and problems about converting between equivalent models - e.g., from regular expressions to nondeterministic finite automata. Moreover, for several problems, this new version also enables teachers and students to automatically generate new problem instances. We also present the results of a survey run on a class of 950 students, which shows very positive results about the usability and usefulness of the tool.

Keywords: Theory of computation · Automata theory · Personalized education · Automata tutor · Automated grading

1 Introduction

Computer science (CS) class enrollments have been rapidly rising, e.g., CS enrollment roughly triples per decade at Berkeley and Stanford [12] or TU Munich.

We thank Emil Ratko-Dehnert from ProLehre TUM for the professional help with the student survey; Tobias Nipkow and his team for allowing us to conduct the user survey in his class; Christian Backs, Vadim Goryainov, Sebastian Mair and Jan Wagener for the exercises they added as part of their Bachelor's theses; Julia Eisentraut and Salomon Sickert-Zehnter for their help in developing this project; the TUM fund "Verbesserung der Lehrmittelsituation" and the CAV community for caring about good teaching. Loris D'Antoni was supported, in part, by NSF under grants CNS-1763871, CCF-1750965, CCF-1744614, and CCF-1704117; and by the UW-Madison OVRGE with funding from WARF.

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Both online and offline courses and degrees are being created to educate students and professionals in computer science and these courses may soon have thousands of students attending a lecture, or tens of thousands following a Massive Online Open Course (MOOC). At these scales, standard approaches to grading and providing personalized feedback are no longer possible and new techniques become both feasible and necessary. Current approaches for handling this growing student volume include reducing the complexity of assignments or relying on imprecise feedback and grading mechanisms. Simpler assessment mechanisms, e.g., multiple-choice questions, are easier to grade automatically but lack realism [8]. Designing better techniques for automated grading and feedback generation is therefore a necessity.

Recent advances in formal methods, including program synthesis and verification, can help teachers and students in verifiably correct ways that statistical or rule-based techniques cannot. For example, formal methods have been used to identify student errors and provide feedback for problems related to introductory Python programming assignments [17] geometry [9,11], algebra [16], logic [2], and automata [3,6]. In particular, for this last topic, the tool Automata Tutor v2 [7] has already been used by more than 9,000 students at more than 30 universities in North America, South America, Europe, and Asia.

In this paper, we present Automata Tutor v3, an online[1] tool that extends Automata Tutor v2 and uses techniques from program synthesis and decision procedures to improve the quality and effectiveness of teaching courses on automata and formal languages. Besides being part of the standard CS curriculum, the concepts taught in these courses are rich in structure and applications, e.g., in control theory, text editors, lexical analyzers, or models of software interfaces. Concrete topics in such curricula include automata, regular expressions, context-free grammars, and Turing machines. For problems and assignments related to these topics Automata Tutor v3 can automatically: (1) Detect whether the student's solution is correct. (2) Detect different types of student's mistakes and translate them into explanatory feedback. (3) If possible, generate new problems together with the corresponding solutions for teachers to use in class.

Automata Tutor v3 greatly expands its predecessor Automata Tutor v2, which only provides ways to pose and solve problems for deterministic and nondeterministic finite automata constructions. This paper describes the new components introduced by Automata Tutor v3 and how this new version improves on its previous one. The key advantages to its competitors are the breadth, automatic generation and grading of exercises, infrastructure allowing for use in large courses and a useful feedback to the students, compared to text-based interfaces used by Autotool [13], rudimentary feedback in JFLAP [14] and none in Gradience [1].

Since Automata Tutor has already been well received by teachers around the world, we believe that the readers from the CAV community will find great value in knowing about this new and fundamentally richer version of the tool and how

[1] https://automata.model.in.tum.de.

it can extensively help with teaching the automata and formal languages courses, a task we know many of the attendees have to face on a yearly basis.

Our contributions are the following:

- **Twelve new types of problems** (added to the four problems from the previous version) that can be created by teachers and for which the *tool can assign grades together with feedback* to student attempts. While the previous version of Automata Tutor could only support problems involving finite automata constructions, Automata Tutor v3 now supports problems for proving language non-regularity using the pumping lemma, building regular expressions, context free grammars, pushdown automata and Turing machines, and conversions between such models.
- **Automatic problem generation** for five types of problems, with the code modularity allowing to add it for all the others. This feature allows teachers to effortlessly create new assignments, or students to practice by themselves with potentially infinitely many exercises.
- A new and **improved user interface** that allows teachers and students to navigate the increased number of problem types and assignments. Furthermore, each problem type comes with an intuitive user interface (e.g., for drawing pushdown automata).
- An improved **infrastructure** for the use in large courses, in particular, incorporating login systems (e.g. *LDAP* or *OAuth*), getting a certified mapping from users to students and enabling teachers to grade homework or exams.
- A **user study** run on a class of 950 students to assess the effectiveness and usability of Automata Tutor v3. In our survey, students report to have *learned quickly*, *felt confident*, and *enjoyed* using Automata Tutor v3, and found it *easy to use*. Most importantly, students found the feedback given by the tool to be *useful* and claimed they *understood more* after using the tool and felt *better prepared* for an upcoming exam. In our personal experience, the tool saves us dozens of thousands of corrections in each single course.

2 Automata Tutor in a Nutshell

Automata Tutor is an online education tool created to support courses teaching basic concepts in automata and formal languages [7]. In this section, we describe how Automata Tutor helps teachers run large courses and students learn efficiently in such courses.

Learning Without Automata Tutor. Figure 1 schematically shows a student-teacher interaction in a course taught without an online tutoring system. The teacher creates exercises, grades them manually, and (sometimes) manually provides personalized feedback to the students. This type of interaction has many limitations: (1) it is asynchronous (i.e., the student has to wait a long time for what is often little feedback) and does not scale to large classrooms, posing strenuous amount of work on teachers, (2) it does not guarantee consistency in the assigned grades and feedback, and (3) it does not allow students to revise

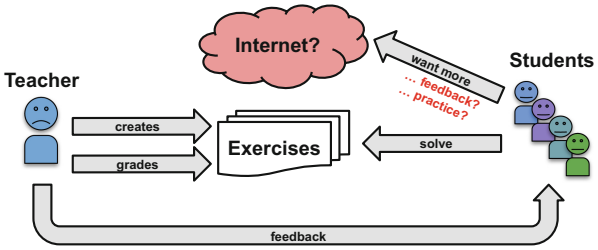

Fig. 1. Common structure of practical sessions for CS classes.

their solutions upon receiving feedback as the teachers often release a solution to all students as part of the feedback and do not grade new submissions.

Another drawback of this interaction is the limited number of problems students can practice on. Because teachers do not have the resources to create many practice problems and provide feedback for them, students are often forced to search the Internet for old exams and practice sheets or even exercises from other universities. Due to the lack of feedback, this chaotic search for practice problems often ends up confusing the students rather than helping them.

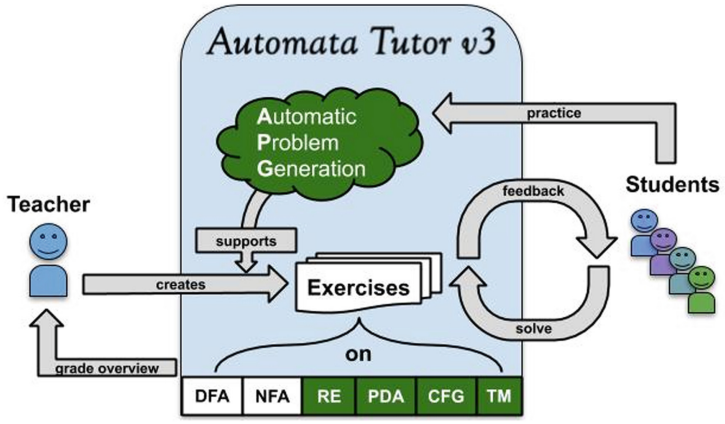

Fig. 2. Overview of Automata Tutor v3 (our contributions in green). The teacher creates exercises on various topics. The students solve the exercises in a feedback cycle: After each attempt they are automatically graded and get personalized feedback. The teacher has access to the grade overview. For additional practice, students can generate an unlimited number of new exercises using the automatic problem generation. (Color figure online)

Learning with Automata Tutor. Figure 2 shows the improved interaction offered by Automata Tutor v3. Here, a teacher creates the problem instances with the

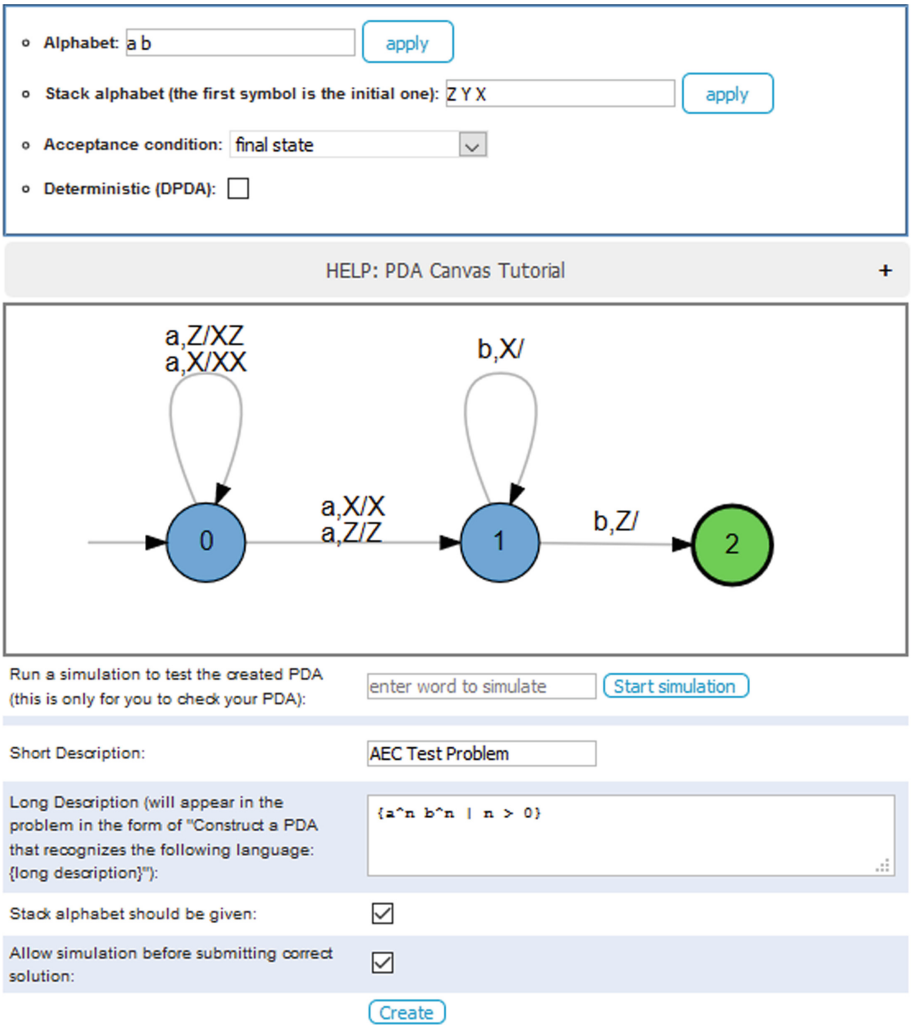

Fig. 3. Creating a new problem of type "PDA Construction".

help of the tool. The problems are then posed to the students and, *no matter how large a class is*, Automata Tutor automatically grades the solution attempts of students right when they are submitted and immediately gives detailed and personalized feedback for each submission. If required, e.g. for a graded homework, it is possible to restrict the number of attempts. Using this feedback, the students can immediately try the problem again and learn from their mistakes. As shown in a large user study run on the first version of Automata Tutor [6], this fast feedback cycle is encouraging for students and results in students spontaneously exploring more practice problems and engaging with the course material. Additional practice is supported by the automatic problem generation, with the

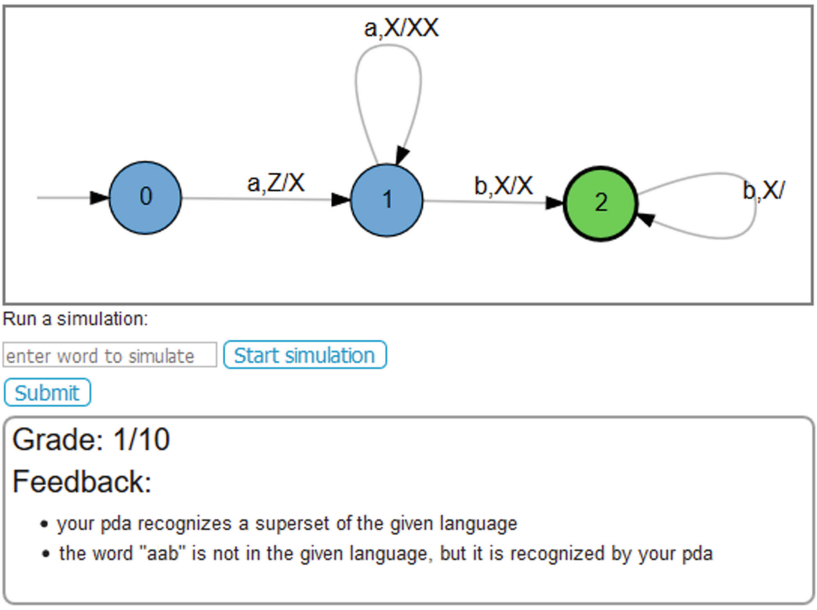

Fig. 4. Feedback received when solving the problem created in Fig. 3.

same level of detailed and personalized feedback as before without increasing the workload of the teacher. Furthermore, automatic problem generation can assist the teacher in creating new exercises. Finally, whenever necessary, the teacher can download an overview of all the grades.

Improved User interface. Automata Tutor is an online tool which runs in the most used browsers. A new collapsible navigation bar groups problems by topic, facilitating quick access to exercises and displaying the structure of the course (see Figure 6 in [5, Appendix B]). To create a new exercise, a teacher clicks the "+"-button and is presented the view of Fig. 3. In this case, the drawing canvas allows to easily specify the sample solution pushdown automaton. Similarly, when students solve this exercise, they draw their solution attempt also on the canvas. After submitting, they receive their personalized feedback and grade (see example in Fig. 4). For the automatic problem generation, a dropdown menu to select the problem type and a slider to select the difficulty is displayed together with the list of all problems the user has generated so far (see the screenshot in Figure 7 in [5, Appendix B]).

3 Design

3.1 University and Course Management

While Automata Tutor can be used for independent online practice, one of the main advantages is its infrastructure for large university courses. To this end,

it is organized in *courses*. A course is created and supervised by one or more teachers. Together, they can create, test and edit exercises. The students cannot immediately see the problems, but only after the teachers have decided to pose them. This involves setting the maximum number of points, the number of allowed attempts as well as the start and end date.

To use Automata Tutor, students must have an account. One can either register by email or, in case the university supports it, login with an external login service like *LDAP* or *Oauth*. When using the login service of their university, teachers get a certified mapping from users to students and enabling teachers to use Automata Tutor v3 for grading homework or exams.

Students can enroll in a course using a password. Enrolled students see all posed problems and can solve them (using the allowed number of attempts). The final grade can be accessed by the teachers in the grade overview.

3.2 New Problem Types

In this section, we list the problem types newly added to Automata Tutor v3. They are all part of the course [10] and a detailed description of each problem can be found in [5, Appendix A], including the basic theoretical concept, how a student can solve such a problem, what a teacher has to provide to create a problem, the idea of the grading algorithm, and what feedback the tool gives.

RE/CFG/PDA Words: Finding words in or not in the language of a regular expression, context free grammar or pushdown automaton.

RE/CFG/PDA Construction: Given a description of a language, construct a regular expression, context free grammar or pushdown automaton.

RE to NFA: Given a regular expression, construct a nondeterministic-finite automaton.

Myhill-Nerode Equivalence Classes: There are two subtypes: either, given a regular expression and two words, find out whether they are equivalent w.r.t. the language, or, given a regular expression and a word, find further words in the same equivalence class.

Pumping-Lemma Game: Given a language, the student has to guess whether it is regular or not and then plays the game as one of the quantifiers.

Find Derivation: Given a context free grammar and a word, the student has to specify a derivation of that word.

CNF: Given a context free grammar, the student has to transform it into Chomsky Normal Form.

CYK: Given a context free grammar in CNF and a word, the student has to decide whether the word is in the language of the grammar by using the Cocke–Younger–Kasami algorithm.

While to TM: Given a while-program (a Turing-complete programming language with very restricted syntax), construct a (multi-tape) Turing machine with the same input-output behaviour.

3.3 Automatic Problem Generation

Automatic Problem Generation (APG) allows one to generate new exercises of a requested *difficulty* level and problem type. This allows students to practice independently and supports teachers when creating new exercises. While APG is currently implemented for four CFG problem types and for the problem type "While to TM", it can be easily extended to other problem types by providing the following components:

- **Procedure for generating exercises at random** either from given basic building blocks or from scratch.
- **A "quality" metric** $qual(E)$ for assessing the quality of the generated exercise E, ranging from trivial or infeasible to realistic.
- **A "difficulty" metric** $diff(E)$ for assessing the difficulty of E.

Given these components, Automata Tutor generates a new problem with a given minimum difficulty $d_{\min}$ and maximum difficulty $d_{\max}$ as follows. Firstly, 100 random exercises are generated. Secondly, Automata Tutor chooses exercises E with the best quality such that $d_{\min} \leq diff(E) \leq d_{\max}$.

Concretely, for the CFG problem types, CFGs with random productions are generated and sanitized. Resulting CFGs that do not accept any words or have too few productions are excluded using the quality metric. The difficulty metric always depends on the number of productions; additionally, depending on the exact problem type, further criteria are taken into account.

For the problem type "While to TM" we use an approach similar to the one suggested in existing tools for automatic problem generation [15,18]: We handcrafted several *base programs* which are of different difficulty level. In the generation process, the syntax tree of such a base program is abstracted and certain modifying operations are executed; these change the program without affecting the difficulty too much. E.g. we choose different variables, switch the order of if-else branches or change arithmetic operators. Then several programs are generated and those of bad quality are filtered out. A program is of bad quality if its language is trivially small or if it contains infinite loops; since detecting these properties is undecidable, we employ heuristics such as checking that the loops terminate for all inputs up to a certain size with a certain timeout.

4 Implementation and Scalability

Automata Tutor v3 is open source and it consists of a frontend, a backend, and a database. It also provides a developer's manual for creating new exercises.

The frontend, written in `scala`, renders the webpage. The drawing canvases for the different automata and the Turing machines rely on javascript. The frontend and backend communicate using XML objects.

The backend, written in C#, contains methods to unpack the xml of the frontend to compute the grade and feedback for solutions. It is also used to check the syntax of exercises and for the automatic problem generation. It relies

on AutomataDotNet[2], a library that provides efficient algorithms for automata and regular expressions.

The database keeps track of existing users, problems and courses. It uses the H2 Database Engine.

All the new parts of Automata Tutor v3 were developed and tested over the last 3 years at TU Munich, where they were used to support the introductory theoretical computer science course. This local deployment served as an important test-bed before publicly deploying the tool online at large scale. Due to its modular structure, the tool is easily scalable by having multiple frontends and backends together with a load distributor. This approach has successfully scaled to 950 concurrent student users; for this, we used 7 virtual machines: 3 hosting frontends, 3 hosting backends (each with 2 cores 2.60 GHz Intel(R) Xeon(R) CPU and 4 GB RAM), and 1 for load distribution and the database (with 4 such cores and 8 GB RAM). We will scale the number of machines based on need.

5 Evaluation and User Study

Large-Class Deployment. In the latest iteration of the TU Munich course in 2019, we used Automata Tutor v3 (in the following denoted as AT) in a mandatory homework system for a course with about 950 students; the homework system also included written and programming exercises. In total, we posed 79 problems consisting of 18 homework and 61 practice problems. The teachers saved themselves the effort of correcting 26,535 homework exercises, and the students used AT to get personalized feedback for their work 76,507 times. On average, each student who used AT did so 107 times.

Student Survey Results. At the end of the course, we conducted an anonymized survey, based on the System Usability Survey [4]. 14.6% of the students in the course answered the survey, which is an ordinary rate of return for an online questionnaire, especially given that there was no incentive. The students were given statements to judge on a Likert scale from 1 to 5 (strongly disagree to strongly agree). We define "The students agreed with the following statement" to mean that the average and median scores were at least 4 and less than 10% of the students chose a score below 3. Dually, if the students disagreed with the statement with median and average score that was at most 2 and less than 10% having a score greater than 3, we say that they "agreed with the negation of the statement". For all statements that do not satisfy either of the criteria, we report mixed answers. The full survey results can be found in [5, Appendix C].

Usability. Regarding the usability of the tool, the students agreed with the following statements:

[2] https://github.com/AutomataDotNet/Automata.

– I quickly learned to use the AT.
– I do *not* need assistance to use the AT.
– I feel confident using the AT.
– The AT is easy to use.
– I enjoy using the AT/the AT is fun to use.

However, there were lots of valuable suggestions for improvements, many of which we have implemented since then. Moreover, the survey also revealed space for improvement, in particular for streamlining as documented by the following statements where the answers were more mixed:

– The AT is unnecessarily complex.
– The canvas for drawing is intuitive.
– The use of AT is self-explanatory.

Usefulness. Regarding how useful AT was for learning, the students agreed with the following statements:

– I understand more after using the AT.
– I prefer using the AT to using pen and paper exercises (12.9% disagreed, but median and average are 4).
– The feedback of the AT was helpful and instructive.
– The exercises within the AT are well-designed.
– The AT fits in well with the programming tasks and written homework.
– The AT did *not* hinder my learning.
– I feel better prepared for the exam after using AT.
– The feedback of the AT was *not* misleading/confusing.

Note that there are no statements with mixed or negative answers regarding the usefulness. Additionally, as shown in Fig. 5, when we asked students about their preferred means of learning, AT gets the highest approval rate, being preferred to written or programming exercises as well as lectures.

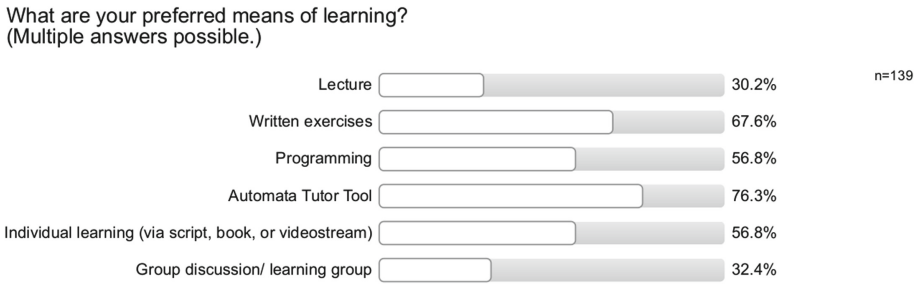

Fig. 5. Question from the survey we conducted to evaluate Automata Tutor, showing that the tool is preferred by a majority of students.

Overall, this class deployment of Automata Tutor v3 and the accompanying surveys were great successes, and showed how the tool is of extreme value for both students and teachers, in particular for such large a course.

6 Conclusion

This paper presents the third version of Automata Tutor, an online tool helping teachers and students in large automata/computation theory courses. Automata Tutor v3 now supports automated grading and feedback generation for a wide variety of problems and, for some of them, even automatic generation of new problem instances. Furthermore, it is easy to extend and we invite the community to contribute by implementing further exercises. Finally, our experience shows that Automata Tutor v3 improves the economical aspects of teaching greatly as it scales effortlessly with the number of students.

Earlier versions of Automata Tutor have already been adopted by thousands of students at dozens of schools and we hope this paper allows Automata Tutor v3 to help even more students and teachers around the world.

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Seminator 2 Can Complement Generalized Büchi Automata via Improved Semi-determinization

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Abstract. We present the second generation of the tool Seminator that transforms transition-based generalized Büchi automata (TGBAs) into equivalent semi-deterministic automata. The tool has been extended with numerous optimizations and produces considerably smaller automata than its first version. In connection with the state-of-the-art LTL to TGBAs translator Spot, Seminator 2 produces smaller (on average) semi-deterministic automata than the direct LTL to semi-deterministic automata translator `ltl2ldgba` of the Owl library. Further, Seminator 2 has been extended with an improved NCSB complementation procedure for semi-deterministic automata, providing a new way to complement automata that is competitive with state-of-the-art complementation tools.

1 Introduction

Semi-deterministic [24] automata are automata where each accepting run makes only finitely many nondeterministic choices. The merit of this interstage between deterministic and nondeterministic automata comes from two facts known since the late 1980s. First, every nondeterministic Büchi automaton with n states can be transformed into an equivalent semi-deterministic Büchi automaton with at most 4^n states [7,24]. Note that asymptotically optimal determinization procedures transform nondeterministic Büchi automata to deterministic automata with $2^{\mathcal{O}(n \log n)}$ states [24] and with a more complex (typically Rabin) acceptance condition, as deterministic Büchi automata are strictly less expressive. Second, some algorithms cannot handle nondeterministic automata, but they can handle semi-deterministic ones; for example, algorithms for qualitative model checking of *Markov decision processes* (MDPs) [7,29].

For theoreticians, the difference between the complexity of determinization and semi-determinization is not dramatic—both constructions are exponential. However, the difference is important for authors and users of practical automata-based tools—automata size and the complexity of their acceptance condition often have a significant impact on tool performance. This latter perspective has recently

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initiated another wave of research on semi-deterministic automata. Since 2015, many new results have been published: several direct translations of LTL to semi-deterministic automata [11,15,16,26], specialized complementation constructions for semi-deterministic automata [4,6], algorithms for quantitative model checking of MDPs based on semi-deterministic automata [13,25], a transformation of semi-deterministic automata to deterministic parity automata [10], and reinforcement learning of control policy using semi-deterministic automata [21].

In 2017, we introduced Seminator 1.1 [5], a tool that transforms nondeterministic automata to semi-deterministic ones. The original semi-determinization procedure of Courcoubetis and Yannakakis [7] works with standard *Büchi automata* (BAs). Seminator 1.1 extends this construction to handle more compact automata, namely *transition-based Büchi automata* (TBAs) and *transition-based generalized Büchi automata* (TGBAs). TBAs use accepting transitions instead of accepting states, and TGBAs have several sets of accepting transitions, each of these sets must be visited infinitely often by accepting runs. The main novelty of Seminator 1.1 was that it performed degeneralization and semi-determinization of a TGBA simultaneously. As a result, it could translate TGBAs to smaller semi-deterministic automata than (to our best knowledge) the only other tool for automata semi-determinization called `nba2ldba` [26]. This tool only accepts BAs as input, and thus TGBAs must be degeneralized before `nba2ldba` is called.

Moreover, in connection with the LTL to TGBAs translator `ltl2tgba` of Spot [8], Seminator 1.1 provided a translation of LTL to semi-deterministic automata that can compete with the direct LTL to semi-deterministic TGBAs translator `ltl2ldba` [26]. More precisely, our experiments [5] showed that the combination of `ltl2tgba` and Seminator 1.1 outperforms `ltl2ldba` on LTL formulas that `ltl2tgba` translates directly to deterministic or semi-deterministic TGBA (i.e., when Seminator has no work to do), while `ltl2ldba` produced (on average) smaller semi-deterministic TGBAs on the remaining LTL formulas (i.e., when the TGBA produced by `ltl2tgba` has to be semi-determinized by Seminator).

This paper presents Seminator 2, which changes the situation. With many improvements in semi-determinization, the combination of `ltl2tgba` and Seminator 2 now translates LTL to smaller (on average) semi-deterministic TGBAs than `ltl2ldba` even for the cases when `ltl2tgba` produces a TGBA that is not semi-deterministic. Moreover, this holds even when we compare to `ltl2ldgba`, which is the current successor of `ltl2ldba` distributed with Owl [19].

Further, Seminator 2 now provides a new feature: *complementation of TGBAs*. Seminator 2 chains semi-determinization with the complementation algorithm called NCSB [4,6], which is tailored for semi-deterministic BAs. Our experiments show that the complementation in Seminator 2 is fully competitive with complementations implemented in state-of-the-art tools [1,8,20,23,30].

2 Improvements in Semi-determinization

First of all, we recall the definition of semi-deterministic automata and principles of the semi-determinization procedure implemented in Seminator 1.1 [5].

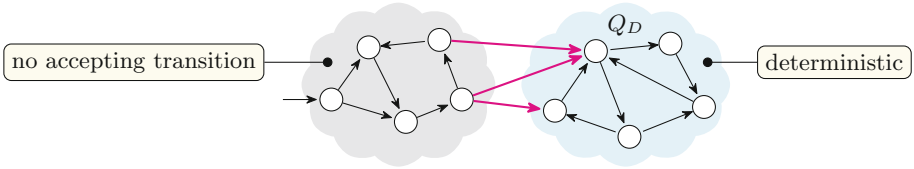

Fig. 1. Structure of a semi-deterministic automaton. The deterministic part contains all accepting transitions and states reachable from them. Cut-transitions are magenta.

Let $\mathcal{A} = (Q, \Sigma, \delta, q_0, \{F_1, \ldots, F_n\})$ be a TGBA over alphabet Σ, with a finite set of states Q, a transition relation $\delta \subseteq Q \times \Sigma \times Q$, an initial state $q_0 \in Q$, and sets of accepting transitions $F_1, \ldots, F_n \subseteq \delta$. Then $\mathcal{A}$ is *semi-deterministic* if there exists a subset $Q_D \subseteq Q$ such that (i) each transition from Q_D goes back to Q_D (i.e., $\delta \cap (Q_D \times \Sigma \times (Q \setminus Q_D)) = \emptyset$), (ii) all states of Q_D are deterministic (i.e., for each $q \in Q_D$ and $a \in \Sigma$ there is at most one q' such that $(q, a, q') \in \delta$), and (iii) each accepting transition starts in a state of Q_D (i.e., $F_1, \ldots, F_n \subseteq Q_D \times \Sigma \times Q_D$).

The part of $\mathcal{A}$ delimited by states of Q_D is called *deterministic*, while the part formed by the remaining states $Q \setminus Q_D$ is called *nondeterministic*, although it could contain deterministic states too. The transitions leading from the nondeterministic part to the deterministic one are called *cut-transitions*. The structure of a semi-deterministic automaton is depicted in Fig. 1.

Intuitively, a TGBA $\mathcal{A}$ with a set of states Q and a single set of accepting transitions F can be transformed into a semi-deterministic TBA $\mathcal{B}$ as follows. First, we use a copy of $\mathcal{A}$ as the nondeterministic part of $\mathcal{B}$. The deterministic part of $\mathcal{B}$ has states of the form (M, N) such that $Q \supseteq M \supseteq N$ and $M \neq \emptyset$. Every accepting transition $(q, a, q') \in F$ induces a cut-transition $(q, a, (\{q'\}, \emptyset))$ of $\mathcal{B}$. The deterministic part is then constructed to track all runs of $\mathcal{A}$ from each such state q' using the powerset construction. More precisely, the first element of (M, N) tracks all runs while the second element tracks only the runs that passed some accepting transition of F. Each transition of the deterministic part, that would reach a state where $M = N$ (so-called *breakpoint*) is replaced with an accepting transition of $\mathcal{B}$ leading to state (M, N'), where N' tracks only the runs of $\mathcal{A}$ passing an accepting transition of F in the current step.

Seminator 1.1 extended this procedure to construct a semi-deterministic TBA even for a TGBA with multiple acceptance sets $F_1, \ldots, F_n$. States of the deterministic part are now triples (M, N, i), where $i \in \{0, \ldots, n-1\}$ is called *level* and it has a similar semantics as in degeneralization. Cut-transitions are induced by transitions of F_n and they lead to states of the form $(\{q'\}, \emptyset, 0)$. The level i says that N tracks runs that passed a transition of F_{i+1} since the last level change. When the deterministic part reaches a state (M, N, i) with $M = N$, we change the level to $i' = (i + 1) \bmod n$ and modify N to track only runs passing $F_{i'+1}$ in the current step. Transitions changing the level are accepting.

A precise description of these semi-determinization procedures and proofs of their correctness can be found in Blahoudek's dissertation [3]. Now we briefly

explain the most important optimizations added in Seminator 2 (we work on a journal paper with their formal description). Each optimization can be enabled/disabled by the corresponding option. All of them are enabled by default.

- `--scc-aware` approach identifies, for each cut-transition, the strongly connected component (SCC) of $\mathcal{A}$ that contains the target of the transition triggering the cut-transition. The sets M, N then track only runs staying in this SCC.
- `--reuse-deterministic` treats in a specific way each deterministic SCC from which only deterministic SCCs are reachable in $\mathcal{A}$: it (i) does not include them in the nondeterministic part, and (ii) copies them (and their successors) in the deterministic part as they are, including the original acceptance transitions. This optimization can result in a semi-deterministic TGBA with multiple acceptance sets on output.
- `--cut-always` changes the policy *when* cut-transitions are created: they are now triggered by all transitions of $\mathcal{A}$ with the target state in an accepting SCC.
- `--powerset-on-cut` applies the powerset construction when computing targets of cut-transitions. The target of a cut-transition leading from q is constructed in the same way as the successor of the hypothetical state $(\{q\}, \emptyset, 0)$ of the deterministic part.
- `--skip-levels` is a variant of the level jumping trick from TGBA degeneralization [2]. Roughly speaking, a single transition in the deterministic part can change the level i directly to $i + j$ where $j \geq 1$ if all runs passed acceptance transitions from all the sets $F_{i+1}, \ldots, F_{i+j}$ in the current step.
- `--jump-to-bottommost` makes sure that all cut-transitions leading to states with the same M component lead to the same state (M, N, i) for some N and i. It relies on the fact that each run takes only one cut-transition, and thus only the component M of the cut-transition's target state is important for determining the acceptance of the run. During the original construction, many states of the form (M, N', i') may appear in different SCCs. After the construction finishes, this optimization redirects each cut-transition leading to (M, N', i') to some state of the form (M, N, i) that belongs to the bottommost SCC (in a topological ordering of the SCCs) that contains such a state. This is inspired by a similar trick used by Křetínský et al. [18] in a different context.
- `--powerset-for-weak` simplifies the construction for weak accepting SCCs (i.e., SCCs where all cycles are accepting) of $\mathcal{A}$. For such SCCs it just applies the powerset construction (builds states of the form M instead of triples (M, N, i)) with all transitions accepting in the deterministic part.

Note that Seminator 1.1 can produce a semi-deterministic TGBA with multiple acceptance sets only when it gets a semi-deterministic TGBA as input. Seminator 2 produces such automata more often due to `--reuse-deterministic`.

3 Implementation and Usage

Seminator 2 is an almost complete rewrite of Seminator [5], and is still distributed under the GNU GPL 3.0 license. Its distribution tarball and source code history

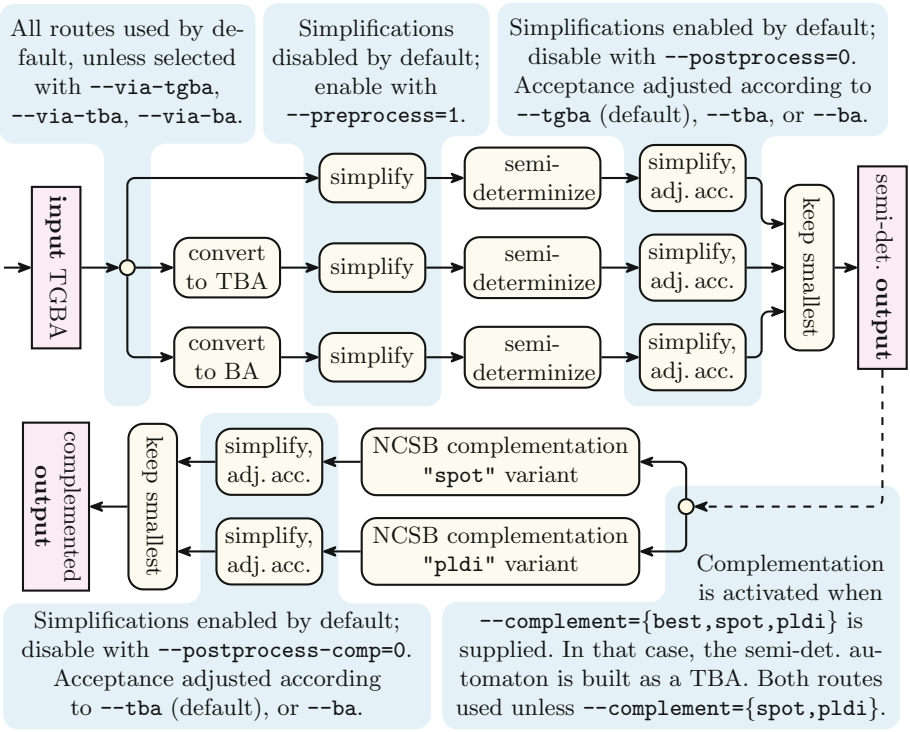

Fig. 2. Workflow for the two operation modes of `seminator`: semi-determinizing and complementing via semi-determinization.

are hosted on GitHub (https://github.com/mklokocka/seminator). The package contains sources of the tool with two user-interfaces (a command-line tool and Python bindings), a test-suite, and some documentation.

Seminator is implemented in C++ on top of the data-structures provided by the Spot library [8], and reuses its input/output functions, simplification algorithms, and the NCSB complementation. The main implementation effort lies in the optimized semi-determinization and an alternative version of NCSB.

The first user interface is a command-line tool called `seminator`. Its high-level workflow is pictured in Fig. 2. By default (top-part of Fig. 2) it takes a TGBA (or TBA or BA) on input and produces a semi-deterministic TGBA (or TBA or BA if requested). Figure 2 details various switches that control the optional simplifications and acceptance transformations that occur before the semi-determinization itself. The pre- and post-processing are provided by the Spot library. The semi-determinization algorithm can be adjusted by additional command-line options (not shown in Fig. 2) that enable or disable optimizations of Sect. 2. As Spot simplification routines are stronger on automata with simpler acceptance conditions, it sometimes pays off to convert the automaton to TBA or BA first. If the input is a TGBA, `seminator` attempts three

semi-determinizations, one on the input TGBA, one on its TBA equivalent, and one on its BA equivalent; only the smallest result is retained. If the input is already a TBA (resp. a BA), only the last two (resp. one) routes are attempted.

The `--complement` option activates the bottom part of Fig. 2 with two variants of the NCSB complementation [4]: `"spot"` stands for a transition-based adaptation of the original algorithm (implemented in Spot); `"pldi"` refers to its modification based on the optimization by Chen et al. [6, Section 5.3] (implemented in Seminator 2). Both variants take a TBA as input and produce a TBA. The options `--tba` and `--ba` apply on the final complement automaton only.

The `seminator` tool can now process automata in batch, making it possible to build pipelines with other commands. For instance the pipeline

```
ltl2tgba <input.ltl | seminator | autfilt --states=3.. >output.hoa
```

uses Spot's `ltl2tgba` command to read a list of LTL formulas from `input.ltl` and transform it into a stream of TGBAs that is passed to `seminator`, which transforms them into semi-deterministic TGBAs, and finally Spot's `autfilt` saves into `output.hoa` the automata with 3 states or more.

Python bindings form the second user-interface and are installed by the Seminator package as an extension of Spot's own Python bindings. It offers several functions, all working with Spot's automata (`twa_graph` objects):

`semi_determinize()` implements the semi-determinization procedure;
`complement_semidet()` implements the `"pldi"` variant of the NCSB complementation for semi-deterministic automata (the other variant is available under the same function name in the bindings of Spot);
`highlight_components()` and `highlight_cut()` provide ways to highlight the nondeterministic and the deterministic parts of a semi-deterministic automaton, and its cut-transitions;
`seminator()` provides an interface similar to the command-line `seminator` tool with options that selectively enable or disable optimizations or trigger complementation.

The Python bindings integrate well with the interactive notebooks of Jupyter [17]. Figure 3 shows an example of such a notebook, using the `seminator()` and `highlight_components()` functions. Additional Jupyter notebooks, distributed with the tool, document the effect of the various optimization options.[1]

4 Experimental Evaluation

We evaluate the performance of Seminator 2 for both semi-determinization and complementation of TGBAs. We compare our tool against several tools listed in Table 1. As `ltl2ldgba` needs LTL on input, we used the set of 221 LTL formulas already considered for benchmarking in the literature [9,12,14,22,27]. To provide TGBAs as input for Seminator 2, we use Spot's `ltl2tgba` to convert the LTL formulas. Based on the automata produced by `ltl2tgba`, we distinguish three

[1] https://nbviewer.jupyter.org/github/mklokocka/seminator/tree/v2.0/notebooks/.

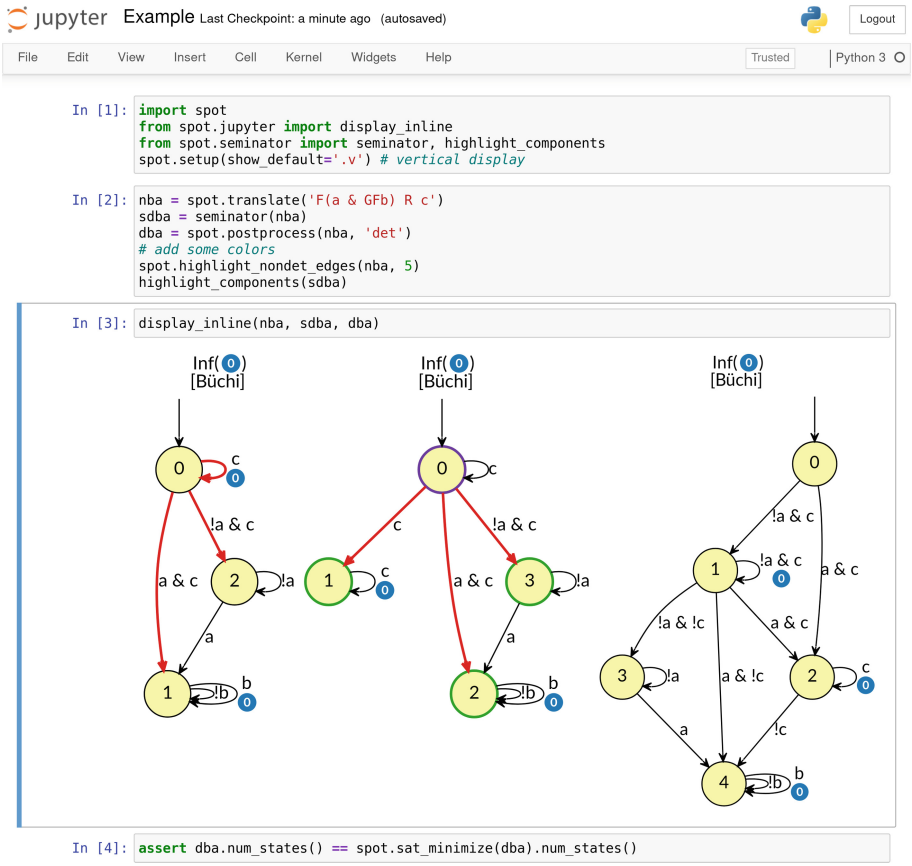

Fig. 3. Jupyter notebook illustrating a case where a nondeterministic TBA (`nba`, left) has an equivalent semi-deterministic TBA (`sdba`, middle) that is smaller than a minimal deterministic TBA (`dba`, right). Accepting transitions are labeled by 0.

categories of formulas: *deterministic* (152 formulas), *semi-deterministic* but not deterministic (49 formulas), and *not semi-deterministic* (20 formulas). This division is motivated by the fact that Seminator 2 applies its semi-determinization only on automata that are not semi-deterministic, and that some complementation tools use different approaches to deterministic automata. We have also generated 500 random LTL formulas of each category.

The scripts and formulas used in those experiments can be found online,[2] as well as a Docker image with these scripts and all the tools installed.[3] All experiments were run inside the supplied Docker image on a laptop Dell XPS13 with Intel i7-1065G7, 16 GB RAM, and running Linux.

[2] https://github.com/xblahoud/seminator-evaluation/.
[3] https://hub.docker.com/r/gadl/seminator.

Table 1. Versions and references to the other tools used in our evaluation.

Package (Tool)	Version	Ref.
Fribourg plugin for GOAL	(na)	[1,30]
GOAL (`gc`)	20200506	[28]
Owl (`ltl2ldgba`)	19.06.03	[11]
ROLL (replaces Buechic)	1.0	[20]
Seminator (`seminator`)	1.1	[5]
Spot (`autfilt`, `ltl2tgba`)	2.9	[8]

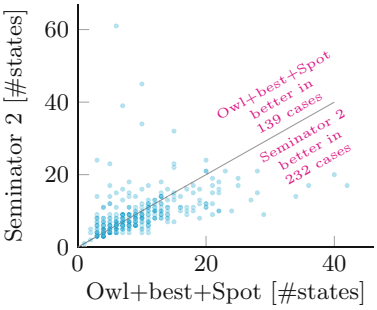

Fig. 4. Comparison of the sizes of the semi-deterministic automata produced by Seminator 2 and Owl for the *not semi-deterministic* random set.

Table 2. Comparison of semi-determinization tools. A benchmark set marked with $x + y$ ⏱ consists of x formulas for which all tools produced some automaton, and y formulas leading to some timeouts. A cell of the form $s\,(m)$ shows the cumulative number s of states of automata produced for the x formulas, and the number m of formulas for which the tool produced the smallest automaton out of the obtained automata. The best results in each column are highlighted.

	(semi-)deterministic		not semi-deterministic	
# of formulas	literature 200+1⏱	random 1000+0⏱	literature 19+1⏱	random 500+0⏱
Owl+best	1092 (102)	6335 (454)	281 (6)	5041 (144)
Owl+best+Spot	978 (139)	5533 (724)	234 (11)	4153 (268)
Seminator 1.1	787 (201)	4947 (963)	297 (7)	7020 (60)
Seminator 2	787 (201)	4947 (963)	230 (16)	3956 (356)

4.1 Semi-determinization

We compare Seminator 2 to its older version 1.1 and to `ltl2ldgba` of Owl. We do not include `Buchifier` [16] as it is available only as a binary for Windows. Also, we did not include `nba2ldba` [26] due to the lack of space and the fact that even Seminator 1.1 performs significantly better than `nba2ldba` [5].

Recall that Seminator 2 calls Spot's automata simplification routines on constructed automata. To get a fair comparison, we apply these routines also to the results of other tools, indicated by *+Spot* in the results. Further, `ltl2ldgba` of Owl can operate in two modes: `--symmetric` and `--asymmetric`. For each formula, we run both settings and pick the better result, indicated by *+best*.

Table 2 presents the cumulative results for each semi-determinization tool and each benchmark set (we actually merged *deterministic* and *semi-deterministic* benchmark sets). The timeout of 30 s was reached by Owl for one formula in

Table 3. Comparison of tools complementing Büchi automata, using the same conventions as Table 2.

	deterministic		semi-detereministic		not semi-deterministic	
# of formulas	literature 147+5⏱	random 500+0⏱	literature 47+2⏱	random 499+1⏱	literature 15+5⏱	random 486+14⏱
ROLL+Spot	1388 (0)	3687 (0)	833 (0)	5681 (4)	272 (0)	6225 (58)
Fribourg+Spot	627 (137)	2493 (464)	290 (26)	3294 (258)	142 (14)	5278 (238)
GOAL+Spot	617 (143)	2490 (477)	277 (28)	3676 (125)	206 (5)	7713 (96)
Spot	611 (150)	2477 (489)	190 (40)	2829 (354)	181 (9)	5310 (202)
Seminator 2	622 (142)	2511 (465)	210 (37)	2781 (420)	169 (8)	4919 (277)

the *(semi-)deterministic* category and by Seminator 1.1 for one formula in the *not semi-deterministic* category. Besides timeouts, the running times of all tools were always below 3 s, with a few exceptions for Seminator 1.1.

In the *(semi-)deterministic* category, the automaton produced by `ltl2tgba` and passed to both versions of Seminator is already semi-deterministic. Hence, both versions of Seminator have nothing to do. This category, in fact, compares `ltl2tgba` of Spot against `ltl2ldgba` of Owl.

Figure 4 shows the distribution of differences between semi-deterministic automata produced by Owl+best+Spot and Seminator 2 for the *not semi-deterministic* random set. A dot at coordinates (x, y) represents a formula for which Owl and Seminator 2 produced automata with x and y states, respectively.

We can observe a huge improvement brought by Seminator 2 in *not semi-deterministic* benchmarks: while in 2017 Seminator 1.1 produced a smaller automaton than Owl in only few cases in this category [5], Seminator 2 is now more than competitive despite the fact that also Owl was improved over the time.

4.2 Complementation

We compare Seminator 2 with the complementation of ROLL based on automata learning (formerly presented as Buechic), the determinization-based algorithm [23] implemented in GOAL, the asymptotically optimal Fribourg complementation implemented as a plugin for GOAL, and with Spot (`autfilt --complement`). We apply the simplifications from Spot to all results and we use Spot's `ltl2tgba` to create the input Büchi automata for all tools, using transition-based generalized acceptance or state-based acceptance as appropriate (only Seminator 2 and Spot can complement transition-based generalized Büchi automata). The timeout of 120 s was reached once by both Seminator 2 and Spot, 6 times by Fribourg, and 13 times by GOAL and ROLL.

Table 3 shows results for complementation in the same way as Table 2 does for semi-determinization. For the *deterministic* benchmark, we can see quite

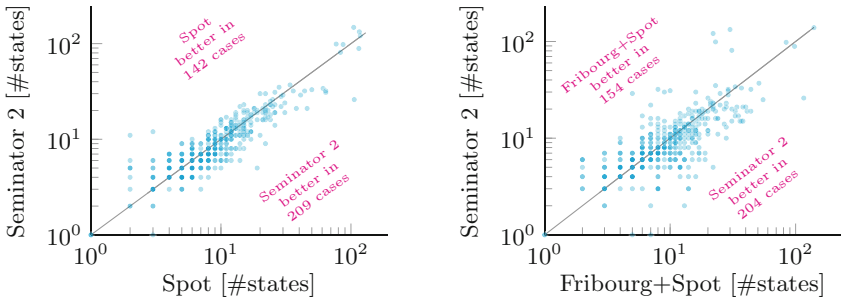

Fig. 5. Comparison of Seminator 2 against Spot and Fribourg+Spot in terms of the sizes (i.e., number of states) of complement automata produced for the *not semi-deterministic* random benchmark. Note that axes are logarithmic.

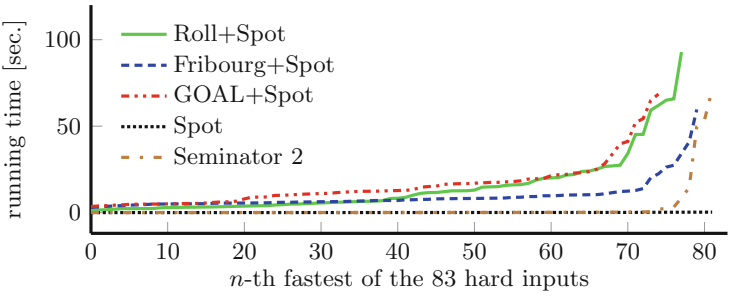

Fig. 6. Running times of complementation tools on the 83 hard cases of the *not semi-deterministic* random benchmark. The running times of each tool on these cases are sorted increasingly before being plotted.

similar results from all tools but ROLL. This is caused by the fact that complementation of deterministic automata is easy. Some tools (including Spot) even apply a dedicated complementation procedure. It comes at no surprise that the specialized algorithm of Seminator 2 performs better than most other complementations in the *semi-deterministic* category. Interestingly, this carries over to the *not semi-deterministic* category. The results demonstrate that the 2-step approach of Seminator 2 to complementation performs well in practice. Figure 5 offers more detailed insight into distribution of automata sizes created by Seminator 2, Spot, and Fribourg+Spot for random benchmarks in this category.

Finally, Fig. 6 compares the running times of these tools over the 83 hard cases of *not semi-deterministic* random benchmark (a case is *hard* if at least one tool did not finish in 10 s). We can see that Seminator 2 and Spot run significantly faster than the other tools.

5 Conclusion

We have presented Seminator 2, which is a substantially improved version of Seminator 1.1. The tool now offers a competitive complementation of TGBA. Furthermore, the semi-determinization code was rewritten and offers new optimizations that significantly reduce the size of produced automata. Finally, new user-interfaces enable convenient processing of large automata sets thanks to the support of pipelines and batch processing, and versatile applicability in education and research thanks to the integration with Spot's Python bindings.

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RTLola Cleared for Take-Off: Monitoring Autonomous Aircraft

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Abstract. The autonomous control of unmanned aircraft is a highly safety-critical domain with great economic potential in a wide range of application areas, including logistics, agriculture, civil engineering, and disaster recovery. We report on the development of a dynamic monitoring framework for the DLR ARTIS (Autonomous Rotorcraft Testbed for Intelligent Systems) family of unmanned aircraft based on the formal specification language RTLola. RTLola is a stream-based specification language for real-time properties. An RTLola specification of hazardous situations and system failures is statically analyzed in terms of consistency and resource usage and then automatically translated into an FPGA-based monitor. Our approach leads to highly efficient, parallelized monitors with formal guarantees on the noninterference of the monitor with the normal operation of the autonomous system.

Keywords: Runtime verification · Stream monitoring · FPGA · Autonomous aircraft

1 Introduction

An unmanned aerial vehicle, commonly known as a drone, is an aircraft without a human pilot on board. While usually connected via radio transmissions to a base station on the ground, such aircraft are increasingly equipped with decision-making capabilities that allow them to autonomously carry out complex missions in applications such as transport, mapping and surveillance, or crop and irrigation monitoring. Despite the obvious safety-criticality of such systems, it is impossible to foresee all situations an autonomous aircraft might encounter and thus make a safety case purely by analyzing all of the potential behaviors in advance. A critical part of the safety engineering of a drone is therefore to carefully monitor the actual behavior during the flight, so that the health status of the system can be assessed and mitigation procedures (such as a return to the base station or an emergency landing) can be initiated when needed.

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In this paper, we report on the development of a dynamic monitoring framework for the DLR ARTIS (Autonomous Rotorcraft Testbed for Intelligent Systems) family of aircraft based on the formal specification language RTLola. The development of a monitoring framework for an autonomous aircraft differs significantly from a monitoring framework in a more standard setting, such as network monitoring. A key consideration is that while the specification language needs to be highly *expressive*, the monitor must operate within strictly limited resources, and the monitor itself needs to be highly *reliable*: any interference with the normal operation of the aircraft could have fatal consequences.

A high level of expressiveness is necessary because the assessment of the health status requires complex analyses, including a cross-validation of different sensor modules such as the agreement between the GPS module and the accelerometer. This is necessary in order to discover a deterioration of a sensor module. At the same time, the expressiveness and the precision of the monitor must be balanced against the available computing resources. The reliability requirement goes beyond pure correctness and robustness of the execution. Most importantly, reliability requires that the peak resource consumption of the monitor in terms of energy, time, and space needs to be known ahead of time. This means that it must be possible to compute these resource requirements statically based on an analysis of the specification. The determination whether the drone is equipped with sufficient hardware can then be made before the flight, and the occurrence of dynamic failures such as running out of memory or sudden drops in voltage can be ruled out. Finally, the collection of the data from the on-board architecture is a non-trivial problem: While the monitor needs access to almost the complete system state, the data needs to be retrieved non-intrusively such that it does not interfere with the normal system operation.

Our monitoring approach is based on the formal stream specification language RTLola [11]. In an RTLola specification, input streams that collect data from sensors, networks, etc., are filtered and combined into output streams that contain data aggregated from multiple sources and over multiple points in time such as over sliding windows of some real-time length. Trigger conditions over these output streams then identify critical situations. An RTLola specification is translated into a monitor defined in a hardware description language and subsequently realized on an FPGA. Before deployment, the specification is checked for consistency and the minimal requirements on the FPGA are computed. The hardware monitor is then placed in a central position where as much sensor data as possible can be collected; during the execution, it then extracts the relevant information. In addition to requiring no physical changes to the system architecture, this integration incurs no further traffic on the bus.

Our experience has been extremely positive: Our approach leads to highly efficient, parallelized monitors with formal guarantees on the non-interference of the monitor with the normal operation of the autonomous system. The monitor is able to detect violations to complex specifications without intruding into the system execution, and operates within narrow resource constraints. RTLola is cleared for take-off.

1.1 Related Work

Stream-based monitoring approaches focus on an expressive specification language while handling non-binary data. Its roots lie in synchronous, declarative stream processing languages like Lustre [13] and Lola [9]. The *Copilot* framework [19] features a declarative data-flow language from which constant space and constant time C monitors are generated; these guarantees enable usage on an embedded device. Rather than focusing on data-flow, the family of Lola-languages puts an emphasis on statistical measures and has successfully been used to monitor synchronous, discrete time properties of autonomous aircraft [1,23]. In contrast to that, RTLola [12,22] supports real-time capabilities and efficient aggregation of data occurring with arbitrary frequency, while forgoing parametrization for efficiency [11]. RTLola can also be compiled to VHDL and subsequently realized on an FPGA [8].

Apart from stream-based monitoring, there is a rich body of monitoring based on real-time temporal logics [2,10,14–16,20] such as Signal Temporal Logic (STL) [17]. Such languages are a concise way to describe temporal behaviors with the shortcoming that they are usually limited to qualitative statements, i.e. boolean verdicts. This limitation was addressed for STL [10] by introducing a quantitative semantics indicating the robustness of a satisfaction. To specify continuous signal patterns, specification languages based on regular expressions can be beneficial, e.g. Signal Regular Expressions (SRE) [5]. The R2U2 tool [18] stands out in particular as it successfully brought a logic closely related to STL onto unmanned aerial systems as an external hardware implementation.

2 Setup

The Autonomous Rotorcraft Testbed for Intelligent Systems (ARTIS) is a platform used by the Institute of Flight Systems of the German Aerospace Center (DLR) to conduct research on autonomous flight. It consists of a set of unmanned helicopters and fixed-wing aircraft of different sizes which can be used to develop new techniques and evaluate them under real-world conditions.

The case study presented in this paper revolves around the superARTIS, a large helicopter with a maximum payload of 85 kg, depicted in Fig. 1. The high payload capabilities allow the aircraft to carry multiple sensor systems, computational resources, and data links. This extensive range of avionic equipment plays an important role in improving the situational awareness of the aircraft [3] during the flight. It facilitates safe autonomous research missions which include flying in urban or maritime areas, alone or with other aircraft. Before an actual flight test, software- and hardware-in-the-loop simulations, as well as real-time logfile replays strengthen confidence in the developed technology.

2.1 Mission

One field of application for unmanned aerial vehicles (UAVs) is reconnaissance missions. In such missions, the aircraft is expected to operate within a fixed area

in which it can cause no harm. The polygonal boundary of this area is called a geo-fence. As soon as the vehicle passes the geo-fence, mitigation procedures need to be initiated to ensure that the aircraft does not stray further away from the safe area.

The case study presented in this paper features a reconnaissance mission. Figure 2 shows the flight path (blue line) within a geo-fence (red line). Evidently, the aircraft violates the fence several times temporarily. A reason for this can be flawed position estimation: An aircraft estimates its position based on several factors such as landmarks detected optically or GPS sensor readings. In the latter case, GPS satellites send position and time information to earth. The GPS module uses this data to compute the aircraft's absolute position with trilateration. However, signal reflection or a low number of GPS satellites in range can result in imprecisions in the position approximation. If the aircraft is continuously exposed to imprecise position updates, the error adds up and results in a strong deviation from the expected flight path.

The impact of this effect can be seen in Fig. 3. It shows the velocity of a ground-borne aircraft in an enclosed backyard according to its GPS module.[1] During the reported period of time, the aircraft was pushed across the backyard by hand. While the expected graph is a smooth curve, the actual measurements show an erratic curve with errors of up to $\pm 1.5\,\mathrm{ms}^{-1}$, which can be mainly attributed to signals being reflected on the enclosure. The strictly positive trend of the horizontal velocity can explain strong deviations from the desired flight path seen in Fig. 3.

A counter-measure to these imprecisions is the cross-validation of several redundant sensors. As an example, rather than just relying on the velocity reported by a GPS module, its measured velocity can be compared to the integrated output of an accelerometer. When the values deviate strongly, the values can be classified as less reliable than when both sensors agree.

2.2 Non-Intrusive Instrumentation

When integrating the monitor into an existing system, the system architecture usually cannot be altered drastically. Moreover, the monitor should not interfere with the regular execution of the system, e.g. by requiring the controller to send explicit messages to it. Such a requirement could offset the timing behavior and thus have a negative impact on the overall performance of the system.

The issue can be circumvented by placing the monitor at a point where it can access all data necessary for the monitoring process non-intrusively. In the case of the superARTIS, the logger interface provides such a place as it compiled the data of all position-related sensors as well as the output of the position estimation [3,4]. Figure 4 outlines the relevant data lines of the aircraft. Sensors were polled with fixed frequencies of up to 100 Hz. The schematic shows that the logger explicitly sends data to the monitor. This is not a strict requirement of

[1] GPS modules only provide absolute position information; the first derivative thereof, however, is the velocity.

Fig. 1. DLR's autonomous superARTIS equipped with optical navigation.

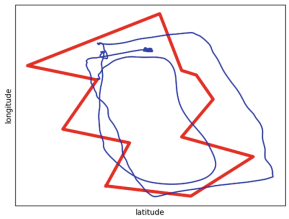


Fig. 2. Reconnaissance mission for a UAV. The thin blue line represents its trajectory, the thick red line a geofence.

the monitor as it could be connected to the data buses leading to the logger and passively read incoming data packets. However, in the present setting, the logger did not run at full capacity. Thus sending information to the monitor came at no relevant cost while requiring few hardware changes to the bus layout.

In turn, the monitor provides feedback regarding violations of the specification. Here, we distinguish between different timing behaviors of triggers. The monitor evaluates event-based triggers whenever the system passes new events to the monitor and immediately replies with the results. For periodic triggers, i.e. , those annotated with an evaluation frequency, the evaluation is decoupled from the communication between monitor and system. Thus, the monitor needs to wait until it receives another event until reporting the verdict. This incurs a short delay between detection and report.

2.3 StreamLAB

StreamLAB[2] [11] is a monitoring framework revolving around the stream-based specification language RTLola. It emphasizes on analyses conducted before deployment of the monitor. This increases the confidence in a successful execution by providing information to aid the specifier. To this end, it detects inconsistencies in the specification such as type errors, e.g. an lossy conversion of a floating point number to an integer, or timing errors, e.g. accessing values that might not exist. Further, it provides two execution modes: an interpreter and an FPGA compilation. The interpreter allows the specifier to validate their specification. For this, it requires a *trace*, i.e. a series of data that is expected to occur during an execution of the system. It then checks whether a trace complies with the specification and reports the points in time when specified bounds are violated. After successfully validating the specification, it can be compiled into VHDL code. Yet again, the compiled code can be analyzed with respect to the space and power consumption. This information allows for evaluating whether the available hardware suffices for running the RTLola monitor.

[2] www.stream-lab.eu.

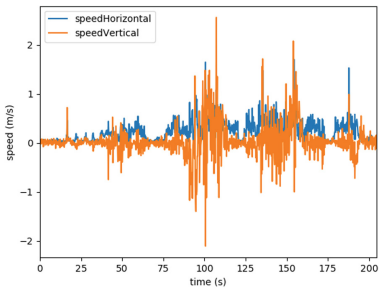


Fig. 3. Line plot of the horizontal and vertical speed calculated by a GPS receiver.

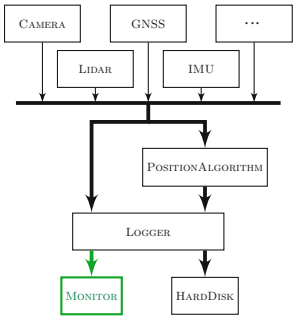


Fig. 4. Overview of data flow in system architecture.

An RTLola specification consists of input and output streams, as well as trigger conditions. *Input* streams describe data the system produces asynchronously and provides to the monitor. *Output* streams use this data to assess the health state of the system e.g. by computing statistical information. *Trigger* conditions distinguish desired and undesired behavior. A violation of the condition issues an alarm to the system.

The following specification declares a floating point input stream `height` representing sensor readings of an altimeter. The output stream `avg_height` computes the average value of the `height` stream over two minutes. The aggregation is a sliding window computed once per second, as indicated with the `@1Hz` annotation.[3] The stream `δheight` computes the difference between the average and the current height. A strong deviation of these values constitutes a suspicious jump in sensor readings, which might indicate a faulty sensor or an unexpected loss or gain in height. In this case, the trigger in the specification issues a warning to the system, which can initiate mitigation measures.

```
input height: Float32
output avg_height @1Hz := height.aggregate(over: 2min, using: avg)
output δheight := abs(avg_height.hold().defaults(to: height) - height)
trigger δheight > 50.0 "WARNING: Suspicious jump in height."
```

Note that this is just a brief introduction to RTLola and the StreamLAB framework. For more details, the authors refer to [8,11,12,22].

2.4 FPGA as Monitoring Platform

An RTLola specification can be compiled into the hardware description language VHDL and subsequently realized on an FPGA as proposed by Baumeister et al. [8]. An FPGA as target platform for the monitor has several advantages

[3] Details on how such a computation can cope with a statically-bounded amount of memory can be found in [12,22].

in terms of improving the development process, reducing its cost, and increasing the overall confidence in the execution.

Since the FPGA is a separate module and thus decoupled from the control software, these components do not share processor time or memory. This especially means that control and monitoring computations happen in parallel. Further, the monitor itself parallelizes the computation of independent RTLola output streams with almost no additional overhead. This significantly accelerates the monitoring process [8]. The compiled VHDL specification allows for extensive static analyses. Most notably, the results include whether the board is sufficiently large in terms of look-up tables and storage capabilities to host the monitor, and the power consumption when idle or at peak performance. Lastly, an FPGA is the sweet spot between generality and specificity: it runs faster, is lighter, and consumes less energy than general purpose hardware while retaining a similar time-to-deployment. The latter combined with a drastically lower cost renders the FPGA superior to application-specific integrated circuits (ASIC) during development phase. After that, when the specification is fixed, an ASIC might be considered for its yet increased performance.

2.5 RTLola Specifications

The entire specification for the mission is comprised of three sub-specifications. This section briefly outlines each of them and explains representative properties in Fig. 5. The complete specifications as well as a detailed description were presented in earlier work [6,21] and the technical report of this paper [7].

Sensor Validation. Sensors can produce incorrect values, e.g. when too few GPS satellites are in range for an accurate trilateration or if the aircraft flies above the range of a radio altimeter. A simple exemplary validation is to check whether the measured altitude is non-negative. If such a check fails, the values are meaningless, so the system should not take them into account in its computations.

Geo-Fence. During the mission, the aircraft has permission to fly inside a zone delimited by a polygon, called a geo-fence. The specification checks whether a face of the fence has been crossed, in which case the aircraft needs to ensure that it does not stray further from the permitted zone.

Sensor Cross-Validation. Sensor redundancy allows for validating a sensor reading by comparing it against readings of other sensors. An agreement between the values raises the confidence in their correctness. An example is the cross-validation of the GPS module against the accelerometer. Integrating the readings of the latter twice yields an absolute position which can be compared against the GPS position.

Figure 5 points out some representative sub-properties of the previously described specification in RTLola, which are too long to discuss them in detail. It contains a validation of GPS readings as well as a cross-validation of the GPS module against the Inertial Measurement Unit (IMU). The specification declares

```
input gps_x: Float16 // Absolute x positive from GPS module
input num_sat : UInt8 // Number of GPS satellites in range
input imu_acc_x: Float32 // Acceleration in x direction from IMU
// Check if the GPS module emitted few readings in the last 3s.
trigger @1Hz gps_x.aggregate(over: 3s, using: count) < 10
  "VIOLATION: Few GPS updates "
// 1 if there are few GPS Satellites in range, otherwise 0.
output few_sat: UInt8 := Int(num_sat < 9)
// Check if there rarely were enough GPS satellites in range.
trigger @1Hz few_sat.aggregate(over: 5s, using: Σ) > 12 "WARNING:
    Unreliable GPS data."
// Integrate acceleration twice to obtain absolute position.
output imu_vel_x@1Hz := imu_acc_x.aggregate(over: ∞, using: ∫)
output imu_x@1Hz := imu_vel_x.aggregate(over: ∞, using: ∫)
// Issue an alarm if readings from GPS and IMU disagree.
trigger abs(imu_x − gps_x) > 0.5 "VIOLATION: GPS and IMU readings
    deviate."
```

Fig. 5. An RTLola specification validating GPS sensor data and cross validating readings from the GPS module and IMU.

three input streams, the x-position and number of GPS satellites in range from the GPS module, and the acceleration in x-direction according to the IMU.

The first trigger counts the number of updates received from the GPS module by counting how often the input stream `gps_x` gets updated to validate the timing behavior of the module.

The output stream `few_sat` computes the indicator function for `num_sat < 9`, which indicates that the GPS module might report unreliable data due to few satellites in reach. If this happens more than 12 times within five seconds, the next trigger issues a warning to indicate that the incoming GPS values might be inaccurate. The last trigger checks whether the double integral of the IMU acceleration coincides with the GPS position up to a threshold of 0.5 m.

2.6 VHDL Synthesis

The specifications mentioned above were compiled into VHDL and realized on the Xilinx ZC702 Base Board[4]. The following table details the resource consumption of each sub-specification reported by the synthesis tool Vivado. The number of flip-flops (FF) indicates the memory consumption in bits; neither specification requires more than 600B of memory. The number of LUTs (Look-up Tables) is an indicator for the complexity of the logic. The sensor validation, despite being significantly longer than the cross-validation, requires the least

[4] https://www.xilinx.com/support/documentation/boards_and_kits/zc702_zvik/ug850-zc702-eval-bd.pdf.

Spec	FF	FF[%]	LUT	LUT[%]	MUX	Idle [mW]	Peak [W]
Geo-fence	2,853	3	26,181	71	4	149	1.871
Validation	4,792	5	34,630	67	104	156	2.085
Cross	3,441	4	23,261	46	99	150	1.911

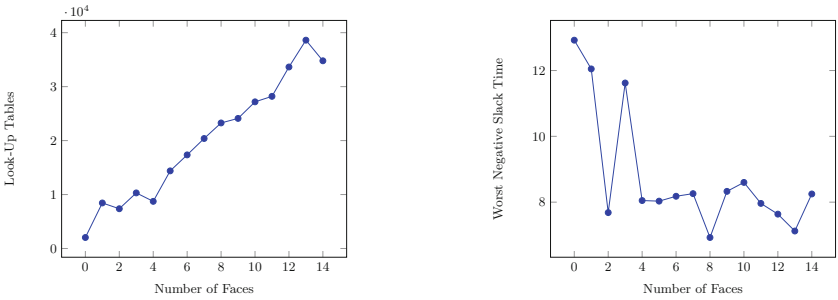
amount of LUTs. The reason is that its computations are simple in comparison: Rather than computing sliding window aggregations or line intersections, it mainly consists of simple thresholding. The number of multiplexers (MUX) reflects this as well: Since thresholding requires comparisons, which translate to multiplexers, the validation requires twice as many of them. Lastly, the power consumption of the monitor is extremely low: When idle, neither specification requires more than 156mW and even under peak pressure, the power consumption does not exceed 2.1W. For comparison, a Raspberry Pi needs between 1.1W (Model 2B) and 2.7W (Model 4B) when idle and roughly twice as much under peak pressure, i.e., 2.1W and 6.4W, respectively.[5]

Note that the geo-fence specification checks for 12 intersections in parallel, one for each face of the fence (cf. Fig. 2). Adapting the number of faces allows for scaling the amount of FPGA resources required, as can be seen in Fig. 6a. The graph does not grow linearly because the realization problem of VHDL code onto an FPGA is a multi-dimensional optimization problem with several pareto-optimal solutions. Under default settings, the optimizer found a solution for four faces that required fewer LUTs than for three faces. At the same time, the worst negative slack time (WNST) of the four-face solution was lower than the WNST for the three-face solution as well (cf. Fig. 6b), indicating that the former performs worst in terms of running time.

3 Results

As the title of the paper suggests, the superARTIS with the RTLola monitor component is cleared to fly and a flight test is already scheduled. In the meantime, the monitor was validated on log files from past missions of the superARTIS replayed under realistic conditions. During a flight, the controller polls samples from sensors, estimates the current position, and sends the respective data to the logger and monitor. In the replay setting, the process remains the same except for one detail: Rather than receiving data from the actual sensors, the data sent to the controller is read from a past log file in the same frequency in which they were recorded. The timing and logging behavior is equivalent to a real execution. This especially means that the replayed data points will be recorded again in the same way. Control computations take place on a machine identical to the one on the actual aircraft. As a result, from the point of view of the monitor, the replay mode and the actual flight are indistinguishable. Note that the setup

[5] Information collected from https://www.pidramble.com/wiki/benchmarks/power-consumption in January, 2020.



(a) Look-Up Tabels (b) Worst Negative Slack Time

Fig. 6. Result of the static analysis for different amounts of face of the geo-fence.

is open-loop, i.e. , the monitor cannot influence the running system. Therefore, the replay mode using real data is more realistic than a high-fidelity simulation.

When monitoring the geo-fence of the reconnaissance mission in Fig. 2, all twelve face crossings were detected successfully. Additionally, when replaying the sensor data of the experiment in the enclosed backyard from Sect. 2.1, the erratic GPS sensor data lead to 113 violations regarding the GPS module on its own. Note that many of these violations point to the same culprit: a low number of available GPS satellites, for example, correlates with the occurrence of peaks in the GPS velocity. Moreover, the cross validation issued another 36 alarms due to a divergence of IMU and GPS readings. Other checks, for example detecting a deterioration of the GPS module based on its output frequency, were not violated in either flight and thus not reported.

4 Conclusion

We have presented the integration of a hardware-based monitor into the superARTIS UAV. The distinguishing features of our approach are the high level of expressiveness of the RTLola specification language combined with the formal guarantees on the resource usage. The comprehensive tool framework facilitates the development of complex specifications, which can be validated on log data before they get translated into a hardware-based monitor. The automatic analysis of the specification derives the minimal requirements on the development board needed for safe operation. If they are met, the specification is realized on an FPGA and integrated into the superARTIS architecture. Our experience shows that the overall system works correctly and reliably, even without thorough system-level testing. This is due to the non-interfering instrumentation, the validated specification, and the formal guarantees on the absence of dynamic failures of the monitor.

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Realizing ω-regular Hyperproperties

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Abstract. We study the expressiveness and reactive synthesis problem of HyperQPTL, a logic that specifies ω-regular hyperproperties. HyperQPTL is an extension of linear-time temporal logic (LTL) with explicit trace and propositional quantification and therefore *truly* combines trace relations and ω-regularity. As such, HyperQPTL can express promptness, which states that there is a common bound on the number of steps up to which an event must have happened. We demonstrate how the HyperQPTL formulation of promptness differs from the type of promptness expressible in the logic Prompt-LTL. Furthermore, we study the realizability problem of HyperQPTL by identifying decidable fragments, where one decidable fragment contains formulas for promptness. We show that, in contrast to the satisfiability problem of HyperQPTL, propositional quantification has an immediate impact on the decidability of the realizability problem. We present a reduction to the realizability problem of HyperLTL, which immediately yields a bounded synthesis procedure. We implemented the synthesis procedure for HyperQPTL in the bounded synthesis tool BoSy. Our experimental results show that a range of arbiter satisfying promptness can be synthesized.

1 Introduction

Hyperproperties [5], which are mainly studied in the area of secure information flow control, are a generalization from trace properties to *sets* of trace properties. That is, they relate multiple execution traces with each other. Examples are noninterference [20], observational determinism [34], symmetry [16], or promptness [24], i.e., properties whose satisfaction cannot be determined by analyzing each execution trace in isolation.

A number of logics have been introduced to express hyperproperties (examples are [4,19,25]). They either add explicit trace quantification to a temporal logic or build on monadic first-order or second-order logics and add an equal-level predicate, which connects traces with each other. A comprehensive study comparing such hyperlogics has been initiated in [6].

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The most prominent hyperlogic is HyperLTL [4], which extends classic linear-time temporal logic (LTL) [26] with trace variables and explicit trace quantification. HyperLTL has been successfully applied in (runtime) verification, (e.g., [15,21,32]), specification analysis [11,14], synthesis [12,13], and program repair [1] of hyperproperties. As an example specification, the following HyperLTL formula expresses observational determinism by stating that for every pair of traces, if the observable inputs I are the same on both traces, then also the observable outputs O have to agree

$$\forall\pi\forall\pi'.\,\square(I_\pi = I_{\pi'}) \rightarrow \square(O_\pi = O_{\pi'}) \ . \tag{1}$$

Thus, hyperlogics can not only specify functional correctness, but may also enforce the absence of information leaks or presence of information propagation. There is a great practical interest in information flow control, which makes synthesizing implementations that satisfy hyperproperties highly desirable. Recently [12], it was shown that the synthesis problem of HyperLTL, although undecidable in general, remains decidable for many fragments, such as the $\exists^*\forall$ fragment. Furthermore, a *bounded synthesis* procedure was developed, for which a prototype implementation based on BoSy [7,9,12] showed promising results.

HyperLTL is, however, intrinsically limited in expressiveness. For example, promptness is not expressible in HyperLTL. Promptness is a property stating that there is a bound b, common for all traces, on the number of steps up to which an event e must have happened. Additionally, just like LTL, HyperLTL can express neither ω-regular nor epistemic properties [2,29]. Epistemic properties are statements about the transfer of knowledge between several components. An exemplary epistemic specification is described by the *dining cryptographers problem* [3]: three cryptographers sit at a table in a restaurant. Either one of the cryptographers or, alternatively, the NSA must pay for their meal. The question is whether there is a protocol where each cryptographer can find out whether the NSA or one of the cryptographers paid the bill, without revealing the identity of the paying cryptographer.

In this paper, we explore HyperQPTL [6,29], a hyperlogic that is more expressive than HyperLTL. Specifically, we study its expressiveness and reactive synthesis problem. HyperQPTL extends HyperLTL with quantification over sequences of new propositions. What makes the logic particularly expressive is the fact that the trace quantifiers and propositional quantifiers can be freely interleaved. With this mechanism, HyperQPTL can not only express all ω-regular properties over a sequences of n-tuples; it truly interweaves trace quantification and ω-regularity. For example, promptness can be stated as the following HyperQPTL formula:

$$\exists b.\forall\pi.\ \diamondsuit b \wedge (\neg b\ \mathcal{U}\, e_\pi) \ . \tag{2}$$

The formula states that there exists a sequence $s \in (2^{\{q\}})^\omega$, such that event e holds on all traces before the first occurrence of b in s. In this paper, we argue that the type of promptness expressible in HyperQPTL is incomparable to the expressiveness of Prompt-LTL [24], a logic introduced to express promptness

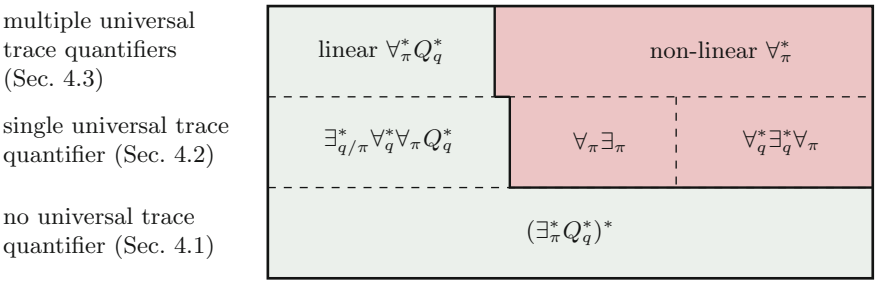


Fig. 1. The realizability problem of HyperQPTL. Left and below of the solid line are the decidable fragments, right above the solid line the undecidable fragments.

properties. It is further known that HyperQPTL also subsumes epistemic extensions of temporal logics such as $\text{LTL}_\mathcal{K}$ [22], as well as the first-order hyperlogic $\text{FO}[<, E]$ [6,19,29]. Its expressiveness makes HyperQPTL particularly interesting. The model checking problem of HyperQPTL is, despite the logic being quite expressive, decidable [29]. We also explore an alternative definition of HyperQPTL that would result in an even more expressive logic. However, we show that the logic would have an undecidable model checking problem, which constitutes a major drawback in the context of computer-aided verification. Furthermore, satisfiability is decidable for large fragments of the logic [6]. Decidable HyperQPTL fragments can be described solely in terms of their *trace* quantifier prefix. This indicates that propositional quantification has no negative impact on the decidability, although it greatly increases the expressiveness. We establish that propositional quantification, in contrast to the satisfiability problem, has an impact on the realizability problem: it becomes undecidable when combining a propositional $\forall\exists$ quantifier alternation with a single universal trace quantifier. However, we show that the synthesis problem of large HyperQPTL fragments remains decidable, where one of these fragments contains promptness properties. We partially obtain these results by reducing the HyperQPTL realizability problem to the HyperLTL realizability problem. Based on this reduction, we extended the BoSy bounded synthesis tool to also synthesize systems respecting HyperQPTL specifications. We provide promising experimental results of our prototype implementation: using BoSy and HyperQPTL specifications, we were able to synthesize arbiters that respect promptness.

This paper is structured as follows. In Sect. 2, we give necessary preliminaries. In Sect. 3, we define HyperQPTL. We discuss an alternative approach to define a logic expressing ω-regular hyperproperties, before pointing out that its model checking problem is undecidable. Subsequently, we give examples for the expressiveness of HyperQPTL, namely by characterizing the type of promptness properties HyperQPTL can express. Additionally, we recapitulate how HyperQPTL also subsumes epistemic properties. Section 4 discusses the realizability problem of HyperQPTL. We describe HyperQPTL fragments in terms of their quantifier prefixes. To present our results, we use the following notation. We write $\forall_\pi$

and $\forall_q$ for a single universal trace and propositional quantifier, respectively. To denote a sequence of universal trace and propositional quantifiers, we write $\forall^*_\pi$ and $\forall^*_q$. Furthermore, we use $\forall^*_{\pi/q}$ for a sequence of mixed universal quantification. We use the analogous notation for existential quantifiers. Lastly, Q^*_π and Q^*_q denote a sequence of mixed universal and existential trace and propositional quantifiers, respectively. As an example, the $\forall^*_\pi Q^*_q$ fragment denotes all formulas of the form $\forall\pi_1 \ldots \forall\pi_m . \exists/\forall q_1 \ldots \exists/\forall q_n . \varphi$, where φ is quantifier free. Figure 1 summarizes our results. We establish that a major factor for the decidability of the realizability problem consists in the number of universal trace occurring in a formula. Realizability of HyperQPTL formulas without $\forall\pi$ quantifiers is decidable (Sect. 4.1). Formulas with a single $\forall\pi$ are decidable if they belong to the $\exists^*_{q/\pi}\forall^*_q\forall_\pi Q^*_q$ fragment. This fragment also contains promptness. For more than one universal trace quantifier, we show that decidability can be guaranteed for a fragment that we call the linear $\forall^*_\pi Q^*_q$ fragment. We also show that all the above fragments are tight, i.e., realizability of all other formulas is in general undecidable. Lastly, Sect. 5 presents experiments for the prototype implementation of our bounded synthesis algorithm for HyperQPTL.

2 Preliminaries

We use AP for a set of atomic propositions. A *trace* over AP is an infinite sequence $t \in (2^{\text{AP}})^\omega$. For $i \in \mathbb{N}$, we write $t[i]$ for the ith element of t and $t[i, \infty]$ for the suffix of t starting from position i. For two traces t, t' over AP and a set AP' $\subseteq$ AP, we write $t =_{\text{AP}'} t'$ to indicate that t and t' agree on all $a \in$ AP', and respectively $T =_{\text{AP}'} T'$ for two sets of traces T and T'. Furthermore, we define a replacement function $t[q \mapsto t_q]$ that given a trace t and a trace $t_q \in (2^{\{q\}})^\omega$, replaces the occurrences of q in t according to t_q, such that $t[q \mapsto t_q] =_{\{q\}} t_q$ and $t[q \mapsto t_q] =_{\text{AP}\setminus\{q\}} t$. We also lift this notation to sets of traces and define $T[q \mapsto t_q] = \{t[q \mapsto t_q] \mid t \in T\}$.

QPTL [31] extends Linear Temporal Logic (LTL) with quantification over propositions. QPTL formulas φ are defined as follows.

$$\varphi ::= \exists q . \varphi \mid \forall q . \varphi \mid \psi$$
$$\psi ::= q \mid \neg\psi \mid \psi \vee \psi \mid \bigcirc\psi \mid \Diamond\psi$$

where $q \in$ AP and AP is a set of atomic propositions. For simplicity, we assume that variable names in formulas are cleared of double occurrences. The semantics of φ over AP is defined with respect to a trace $t \in (2^{\text{AP}})^\omega$.

$$
\begin{array}{lll}
t \models q & \text{iff} & q \in t[0] \\
t \models \neg\psi & \text{iff} & t \not\models \psi \\
t \models \psi_1 \vee \psi_2 & \text{iff} & t \models \psi_1 \text{ or } t \models \psi_2 \\
t \models \bigcirc \psi & \text{iff} & t[1,\infty] \models \psi \\
t \models \Diamond \psi & \text{iff} & \exists i \geq 0.\ t[i,\infty] \models \psi \\
t \models \exists q.\, \varphi & \text{iff} & \exists t_q \in (2^{\{q\}})^\omega.\, t[q \mapsto t_q] \models \varphi \\
t \models \forall q.\, \varphi & \text{iff} & \forall t_q \in (2^{\{q\}})^\omega.\, t[q \mapsto t_q] \models \varphi
\end{array}
$$

We did not define the until operator $\mathcal{U}$ as native part of the logic. It can be derived using propositional quantification [23]. The boolean connectives $\wedge, \rightarrow, \leftrightarrow$ and the temporal operators globally $\Box$ and release $\mathcal{R}$ are derived as usually.

3 ω-Regular Hyperproperties

Just like LTL, HyperLTL cannot express ω-regular languages [29]. LTL can be extended to QPTL by adding quantification over atomic propositions. In QPTL, ω-regular languages become expressible. We therefore study HyperQPTL [6,29], the extension of HyperLTL with propositional quantification, to express ω-regular hyperproperties. Given a set AP of atomic propositions and a set $\mathcal{V}$ of trace variables, the syntax of HyperQPTL is defined as follows

$$
\begin{aligned}
\varphi &::= \forall \pi.\, \varphi \mid \exists \pi.\, \varphi \mid \forall q.\, \varphi \mid \exists q.\, \varphi \mid \psi \\
\psi &::= a_\pi \mid q \mid \neg\psi \mid \psi \vee \psi \mid \bigcirc \psi \mid \Diamond \psi \ ,
\end{aligned}
$$

where $a, q \in \text{AP}$ and $\pi \in \mathcal{V}$. As for QPTL, we assume that formulas are cleared of double occurrences of variable names. We require that in well-defined HyperQPTL formulas, each a_π is in the scope of a trace quantifier binding π and each q is in the scope of a propositional quantifier binding q. Note that atomic propositions a_π refer to a quantified trace π, whereas quantified propositional variables q are independent of the traces. The semantics of a well-defined HyperQPTL formula over AP is defined with respect to a set of traces $T \subseteq (2^{\text{AP}})^\omega$ and an assignment function $\Pi : \mathcal{V} \rightarrow T$. We define the satisfaction relation $\Pi, i \models_T \varphi$ as follows:

$$
\begin{aligned}
&\Pi, i \models_T a_\pi && \text{iff} && a \in \Pi(\pi)[i] \\
&\Pi, i \models_T q && \text{iff} && \forall t \in T.\, q \in t[i] \\
&\Pi, i \models_T \neg\psi && \text{iff} && \Pi, i \not\models_T \psi \\
&\Pi, i \models_T \psi_1 \vee \psi_2 && \text{iff} && \Pi, i \models_T \psi_1 \vee \Pi, i \models_T \psi_2 \\
&\Pi, i \models_T \bigcirc\psi && \text{iff} && \Pi, i+1 \models_T \psi \\
&\Pi, i \models_T \Diamond\psi && \text{iff} && \exists j \geq i.\ \Pi, j \models_T \psi \\
&\Pi, i \models_T \exists\pi.\, \varphi && \text{iff} && \exists t \in T.\, \Pi[\pi \mapsto t], i \models_T \varphi \\
&\Pi, i \models_T \forall\pi.\, \varphi && \text{iff} && \forall t \in T.\, \Pi[\pi \mapsto t], i \models_T \varphi \\
&\Pi, i \models_T \exists q.\, \varphi && \text{iff} && \exists t_q \in (2^{\{q\}})^\omega.\, \Pi, i \models_{T[q \mapsto t_q]} \varphi \\
&\Pi, i \models_T \forall q.\, \varphi && \text{iff} && \forall t_q \in (2^{\{q\}})^\omega.\, \Pi, i \models_{T[q \mapsto t_q]} \varphi\ .
\end{aligned}
$$

Note that the semantics of propositional quantification is defined in such a way that in the scope of a quantifier binding q, all traces agree on their q-sequence. We say that a set of traces T satisfies a HyperQPTL formula φ if $\emptyset, 0 \models_T \varphi$, where $\emptyset$ is the empty trace assignment. QPTL formulas can be expressed in HyperQPTL using a single universal trace quantifier. Furthermore, HyperLTL [4] is the syntactic subset of HyperQPTL that does not contain propositional quantification.

While HyperQPTL can express a wide range of properties (see Sect. 3.1), its model checking problem is still decidable [29]. Furthermore, the syntactic fragments for which satisfiability is decidable can be expressed solely in terms of the occurring trace quantifiers: Just like for HyperLTL, satisfiability of a HyperQPTL formula is decidable if no $\forall\pi$ is followed by an $\exists\pi$ [6].

The definition of HyperQPTL is straightforward, however, one could argue that it is not the only way to extend QPTL to a hyperlogic. The original idea of QPTL is to "color" the trace by introducing additional atomic propositions. The way HyperQPTL is defined, that idea is translated to sets of traces by coloring the traces uniformly. An alternative approach could be to color every trace individually by introducing a full atomic proposition for every propositional quantification. This resembles full second-order quantification and would therefore result in a considerably more expressive logic. In particular, we show that the model checking problem would become undecidable, which is, especially in the context of automatic verification, unfavorable. For the remainder of this section, we call the logic resulting from the alternative definition HyperQPTL$^+$. The syntax of HyperQPTL$^+$ is similar to the one of HyperQPTL, just without the rule q for the evaluation of the propositional variables. This accounts for the idea that the propositional quantification can freely reassign atomic propositions; thus, there is no need to distinguish between free atomic propositions and quantified atomic propositions:

$$
\begin{aligned}
\varphi &::= \forall\pi.\, \varphi \mid \exists\pi.\, \varphi \mid \forall a.\, \varphi \mid \exists a.\, \varphi \mid \psi \\
\psi &::= a_\pi \mid \neg\psi \mid \psi \vee \psi \mid \bigcirc\psi \mid \Diamond\psi\ .
\end{aligned}
$$

Semantically, only the rules for the quantification of the propositional quantifiers change:

$$\begin{aligned} \Pi, i \models_T \exists a.\, \varphi \quad &\text{iff} \quad \exists T' \subseteq (2^{\mathrm{AP}})^\omega.\, T' =_{\mathrm{AP}\setminus\{a\}} T \wedge \Pi, i \models_{T'} \varphi \\ \Pi, i \models_T \forall a.\, \varphi \quad &\text{iff} \quad \forall T' \subseteq (2^{\mathrm{AP}})^\omega.\, T' =_{\mathrm{AP}\setminus\{a\}} T \rightarrow \Pi, i \models_{T'} \varphi \ . \end{aligned}$$

Lemma 1. *The HyperQPTL$^+$ model checking problem is undecidable.*

Proof. Given a finite Kripke structure K and a HyperQPTL$^+$ formula φ, the model checking problem asks whether the trace set T produced by K satisfies φ. The proof follows the undecidability proof for the model checking problem of S1S[E] [6], a logic which lifts S1S to the level of hyperlogics. We describe a reduction from the halting problem of 2-counter machines (which are Turing complete) to the HyperQPTL$^+$ model checking problem. A 2-counter machine (2CM) consists of a finite set of serially numbered instructions that modify two counters. A configuration of a 2CM is a triple $(n, v_1, v_2) \in \mathbb{N}^3$, where n determines the next instruction to be executed, and v_1 and v_2 assign the counter values. Each instruction can either increase or decrease one of the counters; or test either of the counters for zero and, depending on the outcome, jump to another instruction. Furthermore, we assume a special instruction i_{halt}, which indicates that the machine has reached a halting state. A 2CM halts from initial configuration s_0 if there is a finite sequence $s_0, \ldots, s_n$ of configurations such that s_n is a halting configuration and s_{i+1} is a result of applying the instruction in s_i to configuration s_i. Let $\mathcal{M}$ be a 2CM. We describe T and φ such that $T \models \varphi$ iff $\mathcal{M}$ halts. We choose $\mathrm{AP} = \{i, c_1, c_2\}$ and T is the set of all traces where each atomic proposition holds exactly once. That way, a trace t encodes a configuration of the machine: If $i \in t[n]$, $c_1 \in t[v_1]$, and $c_2 \in t[v_2]$, the machine is in configuration (n, v_1, v_2). It is easy to see that T can be produced by a finite Kripke structure. To describe φ, we make two helpful observations. First, using propositional quantification, we can quantify a trace set $T_q \subseteq T$: a trace t is in T_q iff the quantified proposition q eventually occurs on t. Second, for two traces $t, t' \in T$, we can state that t' encodes a configuration which is the successor of the configuration encoded by t. Using these observations, we define $\varphi = \exists q.\, \varphi'$, where q encodes a set $T_q \subseteq T$ that is supposed to describe a halting computation. To ensure that T_q describes a halting computation, φ' is a conjunction of the following requirements: T_q must

1. be finite,
2. contain a halting configuration and the initial configuration,
3. be predecessor closed with respect to the encoded configurations it contains (except for the initial configuration).

Finiteness of T_q can be expressed by stating that there is an upper bound on the values of i, c_1, and c_2 on the traces in T_q. With the observations made before, stating the above requirements in HyperQPTL$^+$ now remains a straightforward exercise. □

Since the model checking problem of HyperQPTL$^+$ is undecidable, we focus on HyperQPTL to express ω-regular hyperproperties. In particular, we show that HyperQPTL can express a range of relevant properties that are neither expressible in HyperLTL, nor in QPTL.

3.1 The Expressiveness of HyperQPTL

HyperQPTL combines trace quantification with ω-regularity. The interplay between the two features enables HyperQPTL to express a variety of properties. In Sect. 1, we showed how HyperQPTL can express a form of promptness. In this section, we further elaborate on the type of properties HyperQPTL can express. In particular, we compare it to Prompt-LTL, a logic that extends LTL with bounded eventualities. Furthermore, HyperQPTL is also able to express epistemic properties by emulating the knowledge operator known from LTL$_\mathcal{K}$.

A straightforward class of properties HyperQPTL can express are ω-regular properties over n-tuples of quantified traces. Formulas expressing this type of properties first have a trace quantifier prefix followed by a QPTL formula, i.e., they lie in the $Q_\pi^* Q_q^*$ fragment. This fragment of HyperQPTL corresponds to the extension of QPTL with *prenex* trace quantification. However, the true expressive power of HyperQPTL originates from the fact that we allow the trace quantifiers and propositional quantifiers to alternate.

Promptness Properties. Promptness properties are an example for HyperQPTL's interplay between trace quantification and propositional quantification. Promptness expresses that eventualities are fulfilled within a bounded number of steps. One way to express promptness properties is the logic Prompt-LTL, which extends LTL with the promptness operator $\diamondsuit_p$. A system satisfies a Prompt-LTL formula φ if there is a bound k such that all traces of the system fulfill the formula where each $\diamondsuit_p$ in φ is replaced by $\diamondsuit^{\leq k}$, i.e., the system must fulfill all prompt eventualities within k steps. For example, $\varphi = \square\diamondsuit_p \psi$ holds in a system if there is a bound k such that all traces of the system at all times satisfy ψ within k steps. HyperQPTL can express a different type of promptness properties. In Sect. 1, Formula 2, we showed how one can state in HyperQPTL that there is a bound, common for all traces, until which an eventuality has to be fulfilled. The idea is to quantify a new proposition b, such that the first position in which b is true serves as the bound. Compared to Prompt-LTL, HyperQPTL thus expresses a weaker form of promptness, while still being stronger than pure eventuality. This type of promptness only becomes meaningful when comparing several traces of the system: HyperQPTL can enforce that there is a common bound for all traces (the system cannot starve), but it does not make the bound explicit. The following example shows a more involved promptness property expressible in HyperQPTL.

Example 1. HyperQPTL can express *bounded waiting for a grant*. It states that if the system requests access to a shared resource at point in time t, then it will be granted access within a bounded amount of time. The bound may depend on

the point in time t where access to the resource was requested. However, it may not depend on the current trace. We express this property in HyperQPTL as follows, also adding that the system will not request access twice without being granted access in between.

$$\forall \pi. \square(r_\pi \rightarrow \bigcirc(\neg r_\pi \mathcal{W}\, g_\pi)) \tag{1}$$

$$\forall \pi. \exists b. \forall \pi'. \square(r_\pi \wedge r_{\pi'} \rightarrow \bigcirc(\diamondsuit b \wedge (\neg b\ \mathcal{U}\, g_\pi) \wedge (\neg b\ \mathcal{U}\, g_{\pi'}))) \tag{2}$$

Formula 1 states that no second request is posed before being given a grant. Formula 2 expresses the bounded waiting property by universally quantifying a trace, then existentially quantifying a sequence of bounds b. Now, for every trace π', whenever π and π' pose a request at the same point in time, both have to get access to the resource before b holds next. Therefore, for each point in time, there is a bound such that all traces posing a request at that point in time get access within a bounded number of steps. Note that this property differs from saying "all traces are eventually granted access", where the bound may also depend on the trace under consideration. In this scenario, each of the infinitely many traces could wait arbitrarily long for the grant. In particular, it could happen that with each trace the waiting time is longer than before.

The above example shows how the interplay of trace quantifiers and propositional quantifiers can be leveraged to express a new class of promptness properties. We finally note that compared to Prompt-LTL, HyperQPTL cannot express that all eventualities must be fulfilled within a fixed k number of steps.

Corollary 1. *The expressiveness of HyperQPTL and Prompt-LTL is incomparable.*

Epistemic Properties. Another interesting class of properties that are not expressible in HyperLTL are epistemic properties. Epistemic properties describe the knowledge of agents that interact with each other in a system. Logics that express epistemic properties are often equipped with a so-called knowledge operator, e.g., $\text{LTL}_\mathcal{K}$, which is LTL extended with the knowledge operator $\mathcal{K}_A\, \varphi$. The operator denotes that an agent $A \subseteq \text{AP}$ knows φ. An agent A is characterized in terms of the atomic propositions he can observe. The semantics of the operator is described with the following rule

$$t, i \models \mathcal{K}_A\, \varphi \quad \text{iff} \quad \forall t'. t[0,i] =_A t'[0,i] \rightarrow t', i \models \varphi \ .$$

The formula is evaluated with respect to a trace t and a position i. We omit the semantic definition for the rest of the logic, which corresponds to plain LTL. The semantic definition of the operator captures the idea that an agent knows some fact φ if φ holds on all traces that are indistinguishable for the agent.

Example 2 (Dining Cryptographers). The dining cryptographers problem [3] is an interesting example of how epistemic properties can characterize non-trivial

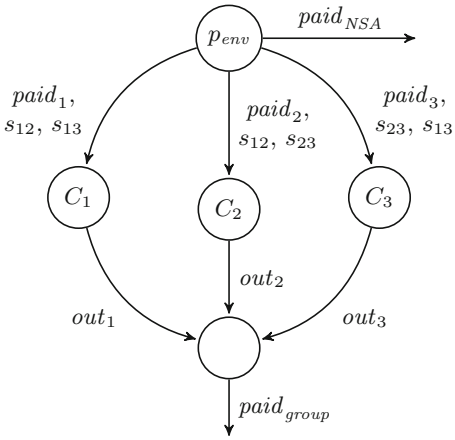


Fig. 2. The dining cryptographers problem with three cryptographers.

protocols. The problem describes the following situation (see Fig. 2): three cryptographers C_1, C_2, and C_3 sit at a table in a restaurant and either one of cryptographers or, alternatively, the NSA paid for their meal. The task for the cryptographers is to figure out whether the NSA or one of the cryptographers paid. However, if one of the cryptographers paid, then the others must not be able to infer who it was. Each cryptographer C_i receives several bits of information: $paid_i$ indicating whether or not he pays the bill, and two secrets, each shared with one of the other cryptographers. The secrets can be used to encode the information they share as output out_i. By combining the outputs of all cryptographers, it must become clear whether the NSA or one of the group paid. The specification of the protocol can be easily formalized in $\text{LTL}_{\mathcal{K}}$. The following formula describes the desired behavior of agent C_1:

$$
\begin{aligned}
&DC\,agent1 := \\
&\quad (paid_{group} \wedge \neg paid_1 \rightarrow (\mathcal{K}_{C_1}(paid_2 \vee paid_3) \wedge \neg \mathcal{K}_{C_1}\, paid_2 \wedge \neg \mathcal{K}_{C_1}\, paid_3)) \\
&\wedge\ (paid_{NSA} \rightarrow \mathcal{K}_{C_1}(\neg paid_1 \wedge \neg paid_2 \wedge \neg paid_3))\ .
\end{aligned}
$$

The knowledge operator can also be defined for hyperlogics [29]. It receives an additional parameter π, indicating the trace the knowledge refers to. When added to HyperQPTL, it has the following semantics:

$$
\Pi, i \models_T \mathcal{K}_{A,\pi}\varphi \qquad \text{iff} \qquad \forall t' \in T.\, \Pi(\pi)[0,i] =_A t'[0,i] \rightarrow \Pi[\pi \mapsto t'], i \models_T \varphi\ .
$$

The knowledge operator, however, can be encoded in HyperQPTL using propositional quantification. Epistemic problems, such as the dining cryptographers problem, can thus be expressed in HyperQPTL.

Theorem 1 (*[29]*). *HyperQPTL can emulate the knowledge operator.*

Proof. We recap the proof from [29]: Let $\varphi = Q_{\pi/q} \dots Q_{\pi/q}.\, \varphi'$ be a HyperQPTL formula, equipped with the knowledge operator as defined above. We assume that φ is given in negated normal form, i.e. each $\mathcal{K}_{A,\pi}$ occurs either in positive position or in negated form. Let u and t be fresh propositions and let π' be a fresh trace variable. Recursively, we replace each knowledge operator $\mathcal{K}_{A,\pi}$ occurring in φ in positive position with the following formula

$$Q_{\pi/q} \dots Q_{\pi/q}.\, \exists u.\, \forall r.\, \forall \pi'.\ \varphi'[\mathcal{K}_{A,\pi}\psi \mapsto u] \wedge \\ ((r\ \mathcal{U}\ (u \wedge r \wedge \bigcirc\Box\neg r)) \wedge \Box(r \rightarrow A_\pi = A_{\pi'}) \rightarrow \Box(r \wedge \bigcirc\neg r \rightarrow \psi[\pi \mapsto \pi']))$$

and each $\mathcal{K}_{A,\pi}$ occurring negatively with the following formula

$$Q_{\pi/q} \dots Q_{\pi/q}.\, \exists u.\, \forall r.\, \exists \pi'.\ \varphi'[\neg\mathcal{K}_{A,\pi}\psi \mapsto u] \wedge \\ ((r\ \mathcal{U}\ (u \wedge r \wedge \bigcirc\Box\neg r)) \rightarrow \Box(r \rightarrow A_\pi = A_{\pi'}) \wedge \Box(r \wedge \bigcirc\neg r \rightarrow \neg\psi[\pi \mapsto \pi'])),$$

where we use $\varphi'[\mathcal{K}_{A,\pi}\psi \mapsto u]$ to denote that in φ', *a single* occurrence of the knowledge operator is replaced by u, and $\psi[\pi \mapsto \pi']$ to denote the formula where π is replaced by π'. The existentially quantified proposition u indicates the points in time where the knowledge operator is supposed to hold/not hold. The universally quantified proposition r is assumed to change once from r to $\neg r$ and thereby point at one of the points in time picked by u. It is then used to compare the prefix of the old trace π and an alternative trace quantified by the trace variable π'. □

4 HyperQPTL Realizability

In reactive synthesis, the task is, given a specification φ, to construct a system that satisfies the specification. More precisely, the system is assumed to receive some inputs from an environment and has to react with outputs such that the specification is fulfilled. The realizability problem asks for the existence of a so-called *strategy tree*, where the edges are labeled with all possible inputs and the task is to find a function f that labels the nodes with the corresponding outputs. Figure 3 shows a strategy tree for a single input bit i. We define strategies following [12]. Let a set $\text{AP} = I \dot\cup O$ be given. A *strategy* $f\colon (2^I)^* \rightarrow 2^O$ maps sequences of input valuations 2^I to an output valuation 2^O. For an infinite word $w = w_0 w_1 w_2 \dots \in (2^I)^\omega$, the trace corresponding to a strategy f is defined as $(f(\epsilon) \cup w_0)(f(w_0) \cup w_1)(f(w_0 w_1) \cup w_2) \dots \in (2^{I \cup O})^\omega$. For any trace $w = w_0 w_1 w_2 \dots \in (2^{I \cup O})^\omega$ and strategy $f\colon (2^I)^* \rightarrow 2^O$, we lift the set containment operator $\in$ defining that $w \in f$ iff $f(\epsilon) = w_0 \cap O$ and $f((w_0 \cap I) \cdots (w_i \cap I)) = w_{i+1} \cap O$ for all $i \geq 0$. We say that a strategy f satisfies a HyperQPTL formula φ over $\text{AP} = I \dot\cup O$ iff $\{w \mid w \in f\}$ satisfies φ.

With the definition of a strategy at hand, we can define the realizability problem of HyperQPTL formally.

Definition 1 (HyperQPTL Realizability). *A HyperQPTL formula φ over atomic propositions $AP = I \dot\cup O$ is realizable if there is a strategy $f\colon (2^I)^* \rightarrow 2^O$ that satisfies φ.*

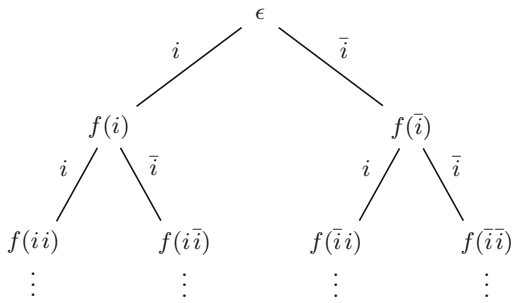


Fig. 3. A strategy tree for the reactive realizability problem.

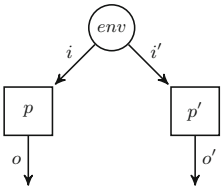
For technical reasons, we assume (without loss of generality) that quantified atomic propositions are classified as outputs, not inputs. This complies with the intuition that propositional quantifiers should be a means for additional expressiveness; they should not overwrite the inputs received from the environment. The definition of realizability of QPTL and HyperLTL specifications is inherited from the definition for HyperQPTL.

Compared to the standard realizability problem, the distributed realizability problem is defined over an architecture, containing a number of processes interacting with each other. The goal is to find a strategy for each of the processes. In the following proofs, we will make use of the distributed realizability problem of QPTL, which we therefore also define formally.

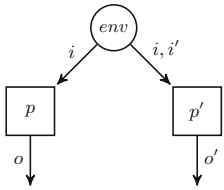
A *distributed architecture* [17,27] A over atomic propositions AP is a tuple $\langle P, p_{env}, \mathcal{I}, \mathcal{O} \rangle$, where P is a finite set of processes and $p_{env} \in P$ is a designated environment process. The functions $\mathcal{I} : P \to 2^{\text{AP}}$ and $\mathcal{O} : P \to 2^{\text{AP}}$ define the inputs and outputs of processes. The output of one process can be the input of another process. The output of the processes must be pairwise disjoint, i.e., for all $p \neq p' \in P$ it holds that $\mathcal{O}(p) \cap \mathcal{O}(p') = \emptyset$. We assume that the environment process forwards inputs to the processes and has no input of its own, i.e., $\mathcal{I}(p_{env}) = \emptyset$.

Definition 2 (Distributed QPTL Realizability *[17]***).** *A QPTL formula φ over free atomic propositions AP is realizable in an architecture $A = \langle P, p_{env}, \mathcal{I}, \mathcal{O} \rangle$ if for each process $p \in P$, there is a strategy $f_p \colon (2^{\mathcal{I}(p)})^* \to 2^{\mathcal{O}(p)}$ such that the combination of all f_p satisfies φ.*

The distributed realizability problem for QPTL is (inherited from LTL) in general undecidable [27]. However, we will use the result that the problem remains decidable for architectures without *information forks*[17]. The notion of information forks captures the flow of data in the system. Intuitively, an architecture contains an information fork if the processes cannot be ordered linearly according to their informedness. Formally, an information fork in an architecture $A = \langle P, p_{env}, \mathcal{I}, \mathcal{O} \rangle$ is defined as a tuple (P', V', p, p'), where p, p' are two different processes, $P' \subseteq P$, and $V' \subseteq AP$ is disjoint from $\mathcal{I}(p) \cup \mathcal{I}(p')$. (P', V', p, p')



(a) Information fork: An architecture with two processes; process p to produces output o from input i and p' produces output o' from input i'.



(b) No information fork: The same architecture as on the left, where the inputs of process p' are changed to i and i'.

Fig. 4. Distributed architectures

is an information fork if P' together with the edges that are labeled with at least one variable from V' forms a subgraph rooted in the environment and there exist two nodes $q, q' \in P'$ that have edges to p, p', respectively, such that $\mathcal{O}(q) \cap \mathcal{I}(p) \not\subseteq \mathcal{I}(p')$ and $\mathcal{O}(q') \cap \mathcal{I}(p') \not\subseteq \mathcal{I}(p)$. The definition formalizes the intuition that p and p' receive incomparable input bits, i.e., they have incomparable information.

Example 3. Two example architectures are depicted in Fig. 4 [12]. The processes in Fig. 4a receive distinct inputs and thus neither process is more informed than the other. The architecture therefore contains an information fork with $P' = \{env, p, p'\}, V' = \{i, i'\}, q = env, q' = env$. The processes in Fig. 4b can be ordered linearly according to the subset relation on the inputs and thus the architecture contains no information fork.

In the following sections, we identify tight syntactic fragments of HyperQPTL for which the standard realizability problem is decidable. We give decidability proofs and show that formulas outside the decidable fragments are in general undecidable. An important aspect for decidability is the number of universal trace quantifiers that appear in the formula. We thus present our findings in three categories, depending on the number of universal trace quantifiers a formula has.

4.1 No Universal Trace Quantifier

We show that the realizability problem of any HyperQPTL formula without a $\forall_\pi$ quantifier is decidable. The problem is reduced to QPTL realizability.

Theorem 2. *Realizability of the $(\exists_\pi^* Q_q^*)^*$ fragment of HyperQPTL is decidable.*

Proof. Let a $(\exists_\pi^* Q_q^*)^*$ HyperQPTL formula φ over $\text{AP} = I \dot\cup O = \{a^0, \ldots, a^k\}$ with trace quantifiers $\pi_0, \ldots \pi_n$ be given. We reduce the problem to the realizability problem of QPTL, which is known to be decidable (since QPTL formulas can be translated to Büchi automata). The idea is to replace each existential trace quantifier $\exists \pi_i$ with quantification of propositions $a^0_{\pi_i}, a^1_{\pi_i}, \ldots, a^k_{\pi_i}$, one for

each $a^j \in \mathrm{AP}$, thereby mimicking the quantification of a trace. To make sure that only traces from an actual strategy tree are chosen, we add a dependency formula which forces the outputs to be dependent on the inputs. The following QPTL formula implements the idea.

$$\varphi_{QPTL} \coloneqq \varphi[i \leq n : \exists \pi_i \mapsto \exists a^0_{\pi_i} \dots \exists a^k_{\pi_i}.] \ \wedge \bigwedge_{i \leq n} \bigwedge_{j \leq n} (I_{\pi_i} \neq I_{\pi_j}) \, \mathcal{R} (O_{\pi_i} = O_{\pi_j})$$

We use the notation $[i \leq n : \exists \pi_i \mapsto \exists a^0_{\pi_i} \dots \exists a^k_{\pi_i}.]$ to indicate that each π_i for $0 \leq i \leq n$ is replaced with the respective series of existential propositional quantification. Furthermore, we write $I_{\pi_i} \neq I_{\pi_j}$ as syntactic sugar for $\bigvee_{a \in I} a_{\pi_i} \nleftrightarrow a_{\pi_j}$ (and similarly for $O_{\pi_i} = O_{\pi_j}$). We show that φ and φ_{QPTL} are equirealizable. For the first direction, assume that φ is realizable by a strategy f. Notice that all atomic propositions in φ_{QPTL} are bound by a propositional quantifier. Therefore, if the witness sequences for the quantified propositions can be chosen correctly, any strategy realizes φ_{QPTL}. Propositions $a^j_{\pi_i}$ are chosen according to the witness traces of $f \models \varphi$. Witnesses for the remaining atomic propositions are also chosen according to their witnesses from $f \models \varphi$. Now, the first conjunct of φ_{QPTL} is fulfilled since $f \models \varphi$ holds. The second conjunct is fulfilled since any two traces π_i, π_j of a strategy tree fulfill by construction $(I_{\pi_i} \neq I_{\pi_j}) \, \mathcal{R} (O_{\pi_i} = O_{\pi_j})$. For the other direction, assume that φ_{QPTL} is realizable (by construction independently from the strategy). Let $t_{a^0_{\pi_0}}, \dots, t_{a^k_{\pi_n}}$ be the witness sequences for the respective quantified atomic propositions. The following strategy realizes φ.

$$f(\sigma) = \begin{cases} \{t_{a_{\pi_i}}[|\sigma|] \mid a \in O\} & \text{if for some } i \leq n, \\ & \quad \sigma = \{t_{a_{\pi_i}}[0] \mid a \in I\} \dots \{t_{a_{\pi_i}}[|\sigma|] \mid a \in I\} \\ \emptyset & \text{otherwise} \end{cases}$$

Strategy f chooses the outputs according to the witnesses for the propositions encoding the traces. Note that because of the second conjunct in φ_{QPTL}, the output is always unique, even if several encoded traces start with the same input sequence. Now, $f \models \varphi$ holds because of the first conjunct of φ_{QPTL}. □

4.2 Single Universal Trace Quantifier

In this fragment, we allow exactly one universal trace quantifier. It is particularly interesting as it contains many promptness properties. For example, the following promptness formulation mentioned in the introduction lies within the fragment:

$$\exists b. \forall \pi. \ \Diamond b \wedge (\neg b \ \mathcal{U} \, e_\pi) \ .$$

Theorem 3. *Realizability of the $\exists^*_{q/\pi} \forall^*_q \forall_\pi Q^*_q$ fragment is decidable.*

We show the theorem in two steps. First, we generalize a proof from [12], showing that realizability of the $\exists^*_\pi \forall_\pi Q^*_q$ fragment is decidable. Second, we show that we can reduce the realizability problem of any HyperQPTL formula to a formula where some propositional quantifiers are replaced with trace quantifiers.

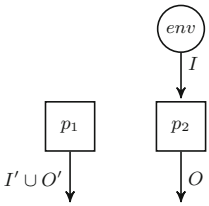


Fig. 5. Distributed architecture encoding existential choice of traces.

Lemma 2. *Realizability of the $\exists^*_\pi \forall_\pi Q^*_q$ fragment is decidable.*

Proof. The reasoning generalizes the proof in [12] showing that realizability $\exists^*_\pi \forall_\pi$ HyperLTL formulas is decidable. We reduce the problem to the distributed realizability problem of QPTL without information forks, which is—since QPTL is subsumed by the μ-calculus—decidable [17]. Let a HyperQPTL formula $\varphi = \exists \pi_1 \dots \exists \pi_n . \forall \pi . \psi$ over $AP = I \dot\cup O$ be given, where ψ is from the Q^*_q fragment. We define a distributed architecture $\mathcal{A}$ over an extended set of atomic propositions $\mathrm{AP}' = I \cup O \cup I' \cup O'$. Similarly to the proof in Theorem 2, I' and O' are composed of a copy of the atomic propositions for each existentially quantified variable π_j. Formally, $I' = \bigcup_{1 \le j \le n} \{ i_{\pi_j} \mid i \in I \}$ and $O' = \bigcup_{1 \le j \le n} \{ o_{\pi_j} \mid o \in O \}$. Now we define $\mathcal{A}$ as follows.

$$\begin{aligned} \mathcal{A} &\coloneqq \langle (p_{env}, p_1, p_2), p_{env}, \mathcal{I}, \mathcal{O}, \rangle \\ \mathcal{I} &\coloneqq (p_1 \mapsto \emptyset, p_2 \mapsto I) \\ \mathcal{O} &\coloneqq (p_{env} \mapsto I, p_1 \mapsto I' \cup O', p_2 \mapsto O) \end{aligned}$$

The architecture is displayed in Fig. 5. The idea is that process p_1 sets the values of all i_{π_j} and o_{π_j} (for $j \le n$) and thereby determines the choice for the existentially quantified traces. Process p_1 receives no input and therefore needs to make a deterministic choice. Process p_2 then solves the realizability of formula $\forall \pi . \psi$. The following QPTL formula φ' encodes the idea.

$$\varphi' \coloneqq \psi' \wedge \Big(\bigwedge_{1 \le j \le n} (I_{\pi_j} \neq I) \, \mathcal{R} (O_{\pi_j} = O) \Big) \ ,$$

where ψ' is defined as ψ, where all a_π are replaced by a (but atomic propositions a_{π_j} are still part of ψ'!). Note that QPTL formulas implicitly quantify over all traces universally. Similarly to the proof in Theorem 2, the second conjunct ensures that process p_1 encodes actual paths from the strategy tree of process p_2 (which is also the strategy tree for formula φ). Thus, φ' is realizable for the distributed architecture $\mathcal{A}$ iff φ is realizable. □

To state the second lemma, we need to define what it means to replace quantifiers in a formula. Let $\varphi = Q_{\pi/q}, \dots, Q_{\pi/q} . \psi$ be a HyperQPTL formula, and J be a set of indices such that for all $j \in J$, there exists a propositional quantifier

$\exists q_j$ or $\forall q_j$ in φ. Furthermore, assume that no π_j with $j \in J$ occurs in φ and that $a \in \text{AP}$. We denote by $\varphi[J \hookrightarrow_a \pi]$ the formula where each propositional quantifier $\exists q_j$ (or $\forall q_j$, respectively) with $j \in J$ is replaced with the corresponding trace quantifier $\exists \pi_j$ (or $\forall \pi_j$, respectively); and each q_j in ψ is replaced by a_{π_j}.

Lemma 3. *Let any HyperQPTL formula φ over $AP = I \dot\cup O$ and a set of indices J be given. If $\varphi[J \hookrightarrow_i \pi]$ is realizable, then so is φ, where $i \in I$ is an arbitrary input, assuming w.l.o.g., that I is non-empty.*

Proof. Let φ and J be given. Formula $\varphi[J \hookrightarrow_i \pi]$ replaces the quantification over sequences $(2^{\{q\}})^\omega$ with trace quantification, where the trace is only used for statements about a single input i. We thus exploit the fact that in the realizability problem, there is a trace for every input sequence. Therefore, the transformed formula is equirealizable. □

Now, we have everything we need to prove Theorem 3.

Proof (of Theorem 3). Let φ be a HyperQPTL formula of the $\exists^*_{q/\pi} \forall^*_q \forall_\pi Q^*_q$ fragment. First, observe that in the quantifier prefix of φ, the $\forall^*_q$ quantifiers and the $\forall_\pi$ can be swapped. The resulting formula belongs to the $\exists^*_{q/\pi} \forall_\pi Q^*_q$ fragment. By Lemma 3, the formula can be transformed to a equirealizable formula of the $\exists^*_\pi \forall_\pi Q^*_q$ fragment, for which realizability is decidable by Lemma 2. □

Lemma 3 allows us to decide realizability of a HyperQPTL formula by replacing propositional quantifiers with trace quantifiers. Thus, we can reduce HyperQPTL realizability to HyperLTL realizability, a fact that we use in Sect. 5 to describe a bounded synthesis algorithm for HyperQPTL.

Corollary 2. *The realizability problem of HyperQPTL can be soundly reduced to the realizability problem of HyperLTL.*

Lastly, we show that the decidable fragment is tight in the class of formulas with a single universal trace quantifier. We do so by showing that a propositional $\forall^*_q \exists^*_q$ quantifier alternation followed by a single trace quantifier $\forall_\pi$ leads to an undecidable realizability problem. The proof is carried out by a reduction from Post's Correspondence Problem.

Theorem 4. *Realizability is undecidable for HyperQPTL formulas with a single $\forall_\pi$ quantifier outside the $\exists^*_{q/\pi} \forall^*_q \forall_\pi Q^*_q$ fragment.*

Proof. Inherited from HyperLTL, realizability of formulas with a $\forall_\pi$ quantifier followed by an $\exists_\pi$ quantifier is undecidable [12]. It remains to show that realizability of formulas from the $\forall^*_q \exists^*_q \forall_\pi$ fragment is in general undecidable. We give a reduction from Post's Correspondence Problem (PCP) [28] to a HyperQPTL formula from the $\forall^*_q \exists^*_q \forall_\pi$ fragment. In PCP, we are given two equally long lists α and β consisting of finite words from some alphabet Σ of size n. PCP is the problem to find an index sequence $(i_k)_{1 \le k \le K}$ with $K \ge 1$ and $1 \le i_k \le n$, such that $\alpha_{i_1} \dots \alpha_{i_K} = \beta_{i_1} \dots \beta_{i_K}$. Intuitively, PCP is the problem of choosing an infinite sequence of domino stones (with finitely many different stones), where each stone

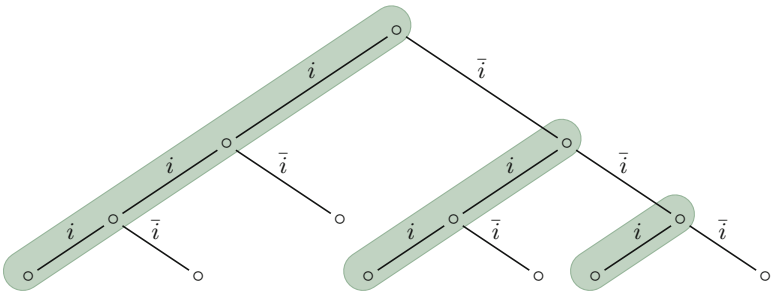


Fig. 6. A sketch of the strategy tree of our PCP reduction: relevant traces are marked in green. (Color figure online)

consists of two words α_i and β_i. Let a PCP instance with $\Sigma = \{a_1, a_2, ..., a_n\}$ and two lists α and β be given. We choose our set of atomic propositions as follows: $\text{AP} \coloneqq I \dot{\cup} O$ with $I \coloneqq \{i\}$ and $O \coloneqq (\Sigma \cup \{\dot{a}_1, \dot{a}_2, ..., \dot{a}_n\} \cup \#)^2$, where we use the dot symbol to encode that a stone starts at this position of the trace. We write $\tilde{a}$ to denote either a or $\dot{a}$. The single input i spans a binary strategy tree. We encode the PCP instance into a HyperQPTL formula that is realizable if and only if the PCP instance has a solution:

$$\forall q_i.\, \forall \boldsymbol{q}.\, \exists p_i.\, \exists \boldsymbol{p}.\, \forall \pi.\, ((\square \pi = p_i) \rightarrow (\square \pi = \boldsymbol{p})) \wedge ((\square \pi = (q_i, \boldsymbol{q})) \rightarrow \varphi_{reduc}(q_i, \boldsymbol{q}, p_i, \boldsymbol{p}))\ ,$$

where $\boldsymbol{q}$ and $\boldsymbol{p}$ are sequences of universally and existentially quantified propositional variables, such that for each $(o, o') \in O$, there is a $q_{(o,o')} \in \boldsymbol{q}$ and a $p_{(o,o')} \in \boldsymbol{p}$. Together with q_i and p_i for the input i, they simulate a universally and an existentially quantified trace from the model. The notation $\pi = \boldsymbol{q}$ denotes that for every $q_a \in \boldsymbol{q}$, it holds that $a_\pi \leftrightarrow q_a$. As seen before, the premise $(\square \pi = (q_i, \boldsymbol{q}))$ and the conjunct $(\square \pi = p_i) \rightarrow (\square \pi = \boldsymbol{p})$ ensure that the propositions $(q_i, \boldsymbol{q})$ and $(p_i, \boldsymbol{p})$ are chosen to represent actual traces from the model. The universal quantification π thus only ensures that $(q_i, \boldsymbol{q})$ and $(p_i, \boldsymbol{p})$, which are used for the main reduction, are chosen correctly. The reduction is implemented in the formula φ_{reduc} and follows the construction in [10], where it is shown that the satisfiability and realizability problem of HyperLTL are undecidable for a $\forall\exists$ trace quantifier prefix.

$$\varphi_{reduc}(q_i, \boldsymbol{q}, p_i, \boldsymbol{p}) \coloneqq \varphi_{rel}(q_i) \rightarrow \varphi_{is++}(q_i, p_i) \wedge \varphi_{start}(\varphi_{stone\&shift}(\boldsymbol{q}, \boldsymbol{p}), q_i) \wedge \varphi_{sol}(q_i, \boldsymbol{q})$$

- $\varphi_{rel}(q_i) \coloneqq \neg q_i \,\mathcal{U}\, \square q_i$ defines the set of *relevant* traces trough the binary strategy tree (see Fig. 6).
- $\varphi_{is++}(q_i, p_i) \coloneqq (\neg q_i \wedge \neg p_i) \,\mathcal{U}\, (\square q_i \wedge \neg p_i \wedge \bigcirc \square p_i)$ defines that a relevant trace is the direct successor trace of another relevant trace.

- $\varphi_{\text{sol}}(q_i, \boldsymbol{q}) \coloneqq \square q_i \rightarrow ((\bigvee_{i=1}^{n} q_{(\dot{a}_i,\dot{a}_i)}) \wedge (\bigvee_{i=1}^{n} q_{(\tilde{a}_i,\tilde{a}_i)}))\, \mathcal{U} \square q_{(\#,\#)}$ ensures that the path on which globally i holds is a "solution" trace, i.e., encodes the PCP solution sequence.
- $\varphi_{start}(\varphi, q_i) \coloneqq \neg q_i \mathcal{U}(\varphi \wedge \square q_i)$ cuts off an irrelevant prefix until φ starts.
- $\varphi_{stone\&shift}(\boldsymbol{q}, \boldsymbol{p})$ encodes that the trace simulated by $\boldsymbol{q}$ starts with a valid encoding of a stone from the PCP instance and that the trace simulated by $\boldsymbol{p}$ encodes the same trace but with the first stone removed (see [10]).

For example, let α with $\alpha_1 = a$, $\alpha_2 = ab$, $\alpha_3 = bba$, and β with $\beta_1 = baa$, $\beta_2 = aa$ and $\beta_3 = bb$ be given. A possible solution for this PCP instance is be $(3, 2, 3, 1)$, since $bbaabbbaa = i_\alpha = i_\beta$. The full sequence at the trace $\square i$ represents the solution with the outputs

$$(\dot{b}, \dot{b})(b, b)(a, \dot{a})(\dot{a}, a)(b, \dot{b})(\dot{b}, b)(b, \dot{b})(a, a)(\dot{a}, a)(\#, \#)(\#, \#) \dots$$

The next relevant trace, therefore, contains

$$(\dot{a}, \dot{a})(b, a)(\dot{b}, \dot{b})(b, b)(a, \dot{b})(\dot{a}, a)(\#, a)(\#, \#)(\#, \#) \dots$$

Continuing this, the following relevant traces are:

$$(\dot{b}, \dot{b})(b, b)(a, \dot{b})(\dot{a}, a)(\#, a)(\#, \#)(\#, \#) \dots$$
$$(\dot{a}, \dot{b})(\#, a)(\#, a)(\#, \#)(\#, \#) \dots$$
$$(\#, \#)(\#, \#) \dots$$

The relevant traces verify the solution provided on the $\square i$ trace by removing one stone after the other. Thus, the formula is realizable iff the PCP instance has a solution. □

4.3 Multiple Universal Trace Quantifiers

When considering multiple universal trace quantifiers $\forall_\pi^*$, the problem becomes undecidable. This is because in HyperLTL, one can encode distributed architectures – for which the problem is undecidable – directly into the formula without using any propositional quantification [12].

Corollary 3. *Realizability of the $\forall_\pi^*$ fragment is in general undecidable.*

However, we show that the realizability problem for formulas with more than one universal trace quantifier is decidable if we restrict ourselves to formulas in the so-called *linear fragment*, i.e., that does not allow an encoding of a distributed architecture. We define the linear fragment of HyperQPTL, where the definitions are adopted from [12].

Let $A, C \subseteq \text{AP}$. We define that atomic propositions $c \in C$ do solely depend on propositions $a \in A$ as the HyperQPTL formula

$$D_{A \mapsto C} \coloneqq \forall \pi \forall \pi'. \left(\bigvee_{a \in A} (a_\pi \nleftrightarrow a_{\pi'}) \right) \mathcal{R} \left(\bigwedge_{c \in C} (c_\pi \leftrightarrow c_{\pi'}) \right) .$$

We define a *collapse* function, which collapses a HyperQPTL formula with a $\forall^*_\pi$ universal quantifier prefix into a formula with a single $\forall_\pi$ quantifier. Propositional quantifiers are preserved by the operation. Let φ be $\forall\pi_1 \cdots \forall\pi_n.\, Q^*_q.\, \psi$. We define the collapsed formula of φ as $\mathit{collapse}(\varphi) := \forall\pi.\, Q^*_q.\, \psi[\pi_1 \mapsto \pi][\pi_2 \mapsto \pi] \ldots [\pi_n \mapsto \pi]$ where $\psi[\pi_i \mapsto \pi]$ replaces all occurrences of π_i in ψ with π.

Lemma 4. *Either* $\varphi \equiv \mathit{collapse}(\varphi)$ *or* φ *has no equivalent* $\forall^1_\pi.\, Q^*_q$ *formula.*

Proof. The collapse function solely works on the trace quantification mechanism of the HyperQPTL formula, by reducing them to a single universal quantification. The theorem has been proven for $\forall^*$ HyperLTL formulas in [12]. Inner propositional quantification does not interfere with this mechanism, hence, the proof can be carried out identically. □

Now we can formally define the linear $\forall^*_\pi$ fragment. Intuitively, we require that every input-output dependency can be ordered linearly, i.e., we are restricted to linear architectures without information forks (see Example 3).

Definition 3. *Let* $O = \{o_1, \ldots, o_n\}$. *A HyperQPTL formula* φ *is called* linear *if for all* $o_i \in O$ *there is a* $J_i \subseteq I$ *such that* $\varphi \wedge D_{I \mapsto O} \equiv \mathit{collapse}(\varphi) \wedge \bigwedge_{o_i \in O} D_{J_i \mapsto \{o_i\}}$ *and* $J_i \subseteq J_{i+1}$ *for all* $i \leq n$.

This results in the following corollary. Since the universal quantifiers can be collapsed, the resulting problem is the realizability problem of QPTL in a linear architecture, which is decidable [17].

Corollary 4. *Realizability of the linear* $\forall^*_\pi Q^*_q$ *fragment is decidable.*

Remark on Complexities. Our aim was to work out the largest possible fragments for which the realizability problem of HyperQPTL remains decidable. The three fragments for which we could prove decidability all subsume the logic QPTL, for which the realizability problem is known to be non-elementary (already its satisfiability problem is non-elementary [30]). Hence, realizability of the discussed HyperQPTL fragments has a non-elementary lower bound. Finding interesting fragments for which the problem has a more feasible complexity therefore remains an open challenge.

5 Experiments

We have implemented a prototype tool that can solve the HyperQPTL realizability problem using the bounded synthesis approach [18]. More concretely, we extended the HyperLTL synthesis tool BoSy [7,9,12]. Bosy reduces the HyperLTL synthesis problem to a SMT constraint system which is then solved by z3 [8] (for more see [12]). We implemented the reduction of HyperQPTL synthesis to HyperLTL synthesis (Corollary 2) in BoSy, such that the tool can also handle HyperQPTL formulas. We evaluated the tool against a range of

Table 1. Experimental results for prompt arbiter

Instance	Bound on system	Bound on ∃-strategy	Result	Time [sec.]
arbiter-2-prompt	2	1	unsat	<1
	2	2	sat	<1
arbiter-2-full-prompt	3	1	unsat	2.4
	3	2	sat	6.0
arbiter-3-prompt	3	1	unsat	4.2
	3	2	sat	9.5
arbiter-4-prompt	4	1	unsat	97
	4	2	?	TO

benchmarks sets, shown in Table 1. The first column indicates the parameterized benchmark name. The second and third columns indicate the bounds given to the bounded synthesis procedure. The second column is the bound on the size of the system. The newest version of BoSy also bounds the size of the strategy for the existential player, this bound is given in column three. For a detailed explanation of how existential strategies are bounded in BoSy, we refer to [7].

We synthesized a range of resource arbiters. Our benchmark set is parametric in the number of clients that can request access to the shared resource (written arbiter-k-prompt where k is the number of clients in Table 1). Unlike normal arbiters, we require the arbiter to fulfill promptness for some of the clients, i.e., requests must be answered within a bounded number of steps [33]. We state the promptness requirement in HyperQPTL by applying the *alternating-color technique* from [24]. Intuitively, the alternating-color technique works as follows: We quantify a q-sequence that "changes color" between q and $\neg q$. Each change of color is used as a potential bound. Once a request occurs, the grant must be given withing two changes of color. Thus, the HyperQPTL formulation amounts to the following specifications, here exemplary for 2 clients, where we require promptness only for client 1.

$$\forall \pi. \square \neg (g^1_\pi \wedge g^2_\pi) \tag{1}$$

$$\forall \pi. \square (r^2_\pi \rightarrow \diamondsuit g^2_\pi) \tag{2}$$

$$\exists q. \forall \pi. \square\diamondsuit q \wedge \square\diamondsuit \neg q \tag{3}$$

$$\begin{aligned} &\wedge \square(r^1_\pi \rightarrow (q \rightarrow (q \,\mathcal{U}(\neg q \,\mathcal{U}\, g^1_\pi))) \\ &\qquad \wedge (\neg q \rightarrow (\neg q \,\mathcal{U}(q \,\mathcal{U}\, g^1_\pi)))) \\ &\forall \pi.(\neg g^1_\pi \,\mathcal{W}\, r^1_\pi) \wedge (\neg g^2_\pi \,\mathcal{W}\, r^2_\pi) \end{aligned} \tag{4}$$

Formula 1 states mutual exclusion. Formula 2 states that client 2 must be served eventually (but not within a bounded number of steps). Formula 3 states the promptness requirement for client 1. It quantifies an alternating q-sequence, which serves as a sequence of global bounds that must be respected on all traces π. Then, if client 1 poses a request, the grant must be given within two changes of the value of q. Formula 4 is only added in benchmarks named arbiter-k-full-prompt. It specifies that no spurious grants should be given.

BoSy successfully synthesizes prompt arbiter of up to 3 states. For a 4-state prompt arbiter BoSy did not return in reasonable time.

6 Conclusion

We studied the hyperlogic HyperQPTL, which combines the concepts of trace relations and ω-regularity. We showed that HyperQPTL is very expressive, it can express properties like *promptness*, *bounded waiting for a grant*, *epistemic* properties, and, in particular, any *ω-regular* property. Those properties are not expressible in previously studied hyperlogics like HyperLTL. At the same time, we argued that the expressiveness of HyperQPTL is optimal in a sense that a more expressive logic for ω-regular hyperproperties would have an undecidable model checking problem. We furthermore studied the realizability problem of HyperQPTL. We showed that realizability is decidable for HyperQPTL fragments that contain properties like promptness. But still, in contrast to the satisfiability problem, propositional quantification does make the realizability problem of hyperlogics harder. More specifically, the HyperQPTL fragment of formulas with a universal-existential propositional quantifier alternation followed by a single trace quantifier is undecidable in general, even though the projection of the fragment to HyperLTL has a decidable realizability problem. Lastly, we implemented the bounded synthesis problem for HyperQPTL in the prototype tool BoSy. Using BoSy with HyperQPTL specifications, we have been able to synthesize several resource arbiters. The synthesis problem of non-linear-time hyperlogics is still open. For example, it is not yet known how to synthesize systems from specifications given in branching-time hyperlogics like HyperCTL*.

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AdamMC: A Model Checker for Petri Nets with Transits against Flow-LTL

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Abstract. The correctness of networks is often described in terms of the individual data flow of components instead of their global behavior. In software-defined networks, it is far more convenient to specify the correct behavior of packets than the global behavior of the entire network. Petri nets with transits extend Petri nets and Flow-LTL extends LTL such that the data flows of tokens can be tracked. We present the tool AdamMC as the first model checker for Petri nets with transits against Flow-LTL. We describe how AdamMC can automatically encode concurrent updates of software-defined networks as Petri nets with transits and how common network specifications can be expressed in Flow-LTL. Underlying AdamMC is a reduction to a circuit model checking problem. We introduce a new reduction method that results in tremendous performance improvements compared to a previous prototype. Thereby, AdamMC can handle software-defined networks with up to 82 switches.

1 Introduction

In networks, it is difficult to specify correctness in terms of the global behavior of the entire system. Instead, the individual *flow* of components is far more convenient to specify correct behavior. For example, loop and drop freedom can be easily specified for the flow of each packet. Petri nets and LTL lack this local view. Petri nets with transits and Flow-LTL have been introduced to overcome this restriction [10]. A transit relation is introduced to follow the *flow* induced by tokens. *Flow-LTL* is a temporal logic to specify both the *local* flow of data and the *global* behavior of markings. The global behavior as in Petri nets and LTL is still important for maximality and fairness assumptions. In this paper,

[1] AdamMC is available online at https://uol.de/en/csd/adammc [12].

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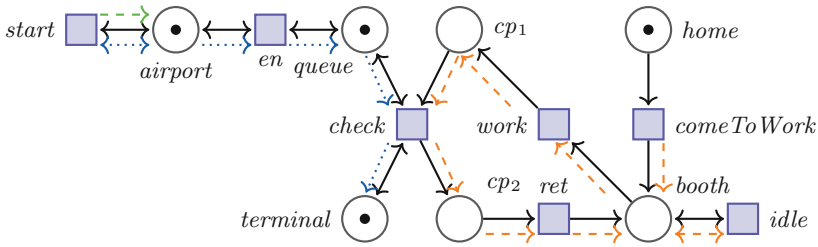

Fig. 1. Access control at an airport modeled as Petri net with transits. Colored arrows display the transit relation and define flow chains to model the passengers.

we present the tool AdamMC[1] as the first model checker for Petri nets with transits against Flow-LTL and its application to software-defined networking.

In Fig. 1, we present an example of a Petri net with transits that models the security check at an airport where passengers are checked by a security guard. The number of passengers entering the airport is unknown in advance. Rather than introducing the complexity of an infinite number of tokens, we use a fixed number of tokens to model possibly infinitely many *flow chains*. This is done by the transit relation which is depicted with colored arrows.

The left-hand side of Fig. 1 models passengers who want to reach the terminal. There are three tokens in the places *airport*, *queue*, and *terminal*. Thus, transitions *start* and *en* are always enabled. Each firing of *start* creates a new flow chain as depicted by the green arrow. This models a new person arriving at the *airport*. Meanwhile, the double-headed blue arrow maintains all flow chains that are still in place *airport*. Passengers have to *en*ter the *queue* and wait until the security *check* is performed. Therefore, transition *en* continues every flow chain in *airport* to *queue*. Checking the passengers is carried out by transition *check* which becomes enabled if the security guard *work*s. Thus, passengers residing in *queue* have to wait until the guard *check*s them. Afterwards, they reach the *terminal*. The security guard is modeled on the right-hand side of Fig. 1. By firing *comeToWork* and thus moving the token in place *home*, her flow chain starts and she can repeatedly either *idle* or *work*, *check* passengers, and *ret*urn. Her transit relation is depicted in orange and models exactly one flow chain.

In Fig. 1, we define the checkpoints cp_1 and cp_2 and the *booth* as a security zone and require that passengers never enter the security zone and eventually reach the *terminal*. The flow formula $\varphi = \mathbb{A}(\mathit{airport} \rightarrow (\Box\neg(\mathit{cp}_1 \vee \mathit{cp}_2 \vee \mathit{booth}) \wedge \Diamond \mathit{terminal}))$ specifies this. AdamMC verifies the example from Fig. 1 against the formula $\Box\Diamond\, \mathit{check} \rightarrow \varphi$ specifying that if passengers are checked regularly then they cannot access the security zone and eventually reach the terminal.

In this paper, we present AdamMC as a full-fledged tool. First, AdamMC can handle Petri nets with transits and Flow-LTL formulas in general. Second, AdamMC has an input interface for a concurrent update and a software-defined network and encodes both of them as a Petri nets with transits. Common assumptions on fairness and requirements for network correctness are also provided as Flow-LTL formulas. This allows users of the tool to model check the

correctness of concurrent updates and to prevent packet loss, routing loops, and network congestion. Third, AdamMC provides algorithms to check safe Petri nets against LTL with *both* places and transitions as atomic propositions which makes it especially easy to specify fairness and maximality assumptions.

The tool reduces the model checking problem for safe Petri nets with transits against Flow-LTL to the model checking problem for safe Petri nets against LTL. We develop the new *parallel approach* to check global and local behavior in parallel instead of sequentially. This approach yields a tremendous speed-up for a few local requirements and realistic fairness assumptions in comparison to the sequential approach of a previous prototype [10]. In general, the parallel approach has worst-case complexity inferior to the sequential approach even though the complexities of both approaches are the same when using only one flow formula.

As last step, AdamMC reduces the model checking problem of safe Petri nets against LTL to a circuit model checking problem. This is solved by ABC [2,4] with effective verification techniques like IC3 and bounded model checking. AdamMC verifies concurrent updates of software-defined networks with up to 38 switches (31 more than the prototype) and falsifies concurrent updates of software-defined networks with up to 82 switches (44 more than the prototype).

The paper is structured as follows: In Sect. 2, we recall Petri nets with transits and Flow-LTL. In Sect. 3, we outline the three application areas of AdamMC: checking safe Petri nets with transits against Flow-LTL, checking concurrent updates of software-defined networks against common assumptions and specifications, and checking safe Petri nets against LTL. In Sect. 4, we algorithmically encode concurrent updates of software-defined networks in Petri nets with transits. In Sect. 5, we introduce the parallel approach for the underlying circuit model checking problem. In Sect. 6, we present our experimental evaluation.

Further details can be found in the full paper [13].

2 Petri Nets with Transits and Flow-LTL

A safe *Petri net with transits* $\mathcal{N} = (\mathscr{P}, \mathscr{T}, \mathscr{F}, In, \Upsilon)$ [10] contains the set of *places* $\mathscr{P}$, the set of *transitions* $\mathscr{T}$, the *flow relation* $\mathscr{F} \subseteq (\mathscr{P} \times \mathscr{T}) \cup (\mathscr{T} \times \mathscr{P})$, and the *initial marking* $In \subseteq \mathscr{P}$ as in safe Petri nets [27]. In a *safe* Petri net, reachable markings contain at most one token per place. The *transit relation* Υ is for every transition $t \in \mathscr{T}$ of type $\Upsilon(t) \subseteq (pre^{\mathcal{N}}(t) \cup \{\triangleright\}) \times post^{\mathcal{N}}(t)$. With $p\ \Upsilon(t)\ q$, we define that firing transition t *transits* the flow in place p to place q. The symbol $\triangleright$ denotes a *start* and $\triangleright\ \Upsilon(t)\ q$ defines that firing transition t *starts* a new flow for the token in place q. Note that the transit relation can split, merge, and end flows. A sequence of flows leads to a *flow chain* which is a sequence of the current place and the fired outgoing transition. Thus, Petri nets with transits can describe both the global progress of tokens and the local flow of data.

Flow-LTL [10] extends Linear-time Temporal Logic (LTL) and uses places and transitions as atomic propositions. It introduces $\mathbb{A}$ as a new operator which uses LTL to specify the flow of data for *all* flow chains. For Fig. 1, the formula $\mathbb{A}(\mathit{booth} \rightarrow \Diamond\, \mathit{check})$ specifies that the guard performs at least one check. We call

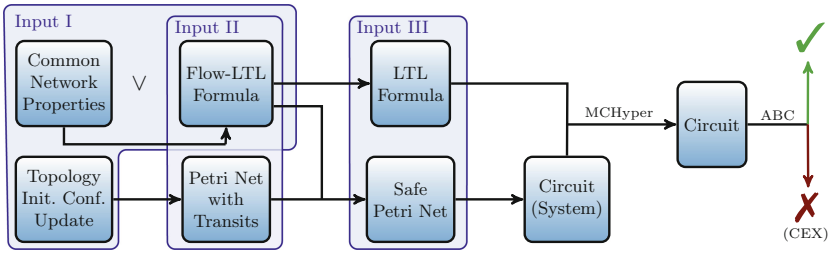

Fig. 2. Overview of the workflow of AdamMC: The application areas of the tool are given by three different input domains: software-defined network/Flow-LTL (Input I), Petri nets with transits/Flow-LTL (Input II), and Petri nets/LTL (Input III). AdamMC performs all unlabeled steps. MCHyper creates the final circuit which ABC checks to answer the initial model checking problem.

formulas starting with $\mathbb{A}$ *flow formulas*. Formulas around flow formulas specify the global progress of tokens in the form of markings and fired transitions to formalize maximality and fairness assumptions. These formulas are called *run formulas*. Often, Flow-LTL formulas have the form *run formula* $\rightarrow$ *flow formula*.

3 Application Areas

AdamMC consists of modules for three application areas: checking safe Petri nets with transits against Flow-LTL, checking concurrent updates of software-defined networks against common assumptions and specifications, and checking safe Petri nets against LTL. The general architecture and workflow of the model checking procedure is given in Fig. 2. AdamMC is based on the tool Adam [14].

Petri Nets with Transits. Petri nets with transits follow the progress of tokens and the flow of data. Flow-LTL allows to specify requirements on both. For Petri nets with transits and Flow-LTL (Input II), AdamMC extends a parser for Petri nets provided by APT [30], provides a parser for Flow-LTL, and implements two reduction methods to create a safe Petri net and an LTL formula. The sequential approach is outlined in [10] and the parallel approach in Sect. 5.

Software-Defined Networks. Concurrent updates of software-defined networks are the second application area of AdamMC. The tool automatically encodes an initially configured network topology and a concurrent update as a Petri net with transits. The concurrent update renews the forwarding table. We provide parsers for the *network topology*, the *initial configuration*, the *concurrent update*, and Flow-LTL (Input I). In Sect. 4, we present the creation of a Petri net with transits from the input and Flow-LTL formulas for *common network properties* like *connectivity*, *loop freedom*, *drop freedom*, and *packet coherence*.

Petri Nets. AdamMC supports the model checking of safe Petri nets against LTL with both places *and* transitions as atomic propositions. It provides dedicated algorithms to check *interleaving-maximal* runs of the system. A run is interleaving-maximal if a transition is fired whenever a transition is

enabled. Furthermore, AdamMC allows a concurrent view on runs and can check *concurrency-maximal* runs which demand that each subprocess of the system has to progress maximally rather than only the entire system. State-of-the-art tools like LoLA [32] and ITS-Tools [29] are restricted to interleaving-maximal runs and places as atomic propositions. For Petri net model checking (Input III), we allow Petri nets in APT and PNML format as input and provide a parser for LTL formulas.

The construction of the circuit in Aiger format [3] is defined in [11]. MCHyper [15] is used to create a circuit from a given circuit and an LTL formula. This circuit is given to ABC [2,4] which provides a toolbox of modern hardware verification algorithms like IC3 and bounded model checking to decide the initial model checking question. As output for all three modules, AdamMC transforms a possible counterexample (CEX) from ABC into a counterexample to the Petri net (with transits) and visualizes the net with Graphviz and the dot language [9]. When no counterexample exists, AdamMC verified the input successfully.

4 Verifying Updates of Software Defined Networks

We show how AdamMC can check concurrent updates of realistic examples from software-defined networking (SDN) against typical specifications [19]. SDN [6,25] separates the *data plane* for forwarding packets and the *control plane* for the routing configuration. A central controller initiates updates which can cause problems like routing loops or packet loss. AdamMC provides an input interface to automatically encode software-defined networks and concurrent updates of their configuration as Petri nets with transits. The tool checks requirements like loop and drop freedom to find erroneous updates before they are deployed.

4.1 Network Topology, Configurations, and Updates

A *network topology* T is an undirected graph $T = (Sw, Con)$ with *switches* as vertices and *connections* between switches as edges. Packets enter the network at *ingress* switches and they leave at *egress* switches. *Forwarding* rules are of the form `x.fwd(y)` with $\mathtt{x}, \mathtt{y} \in Sw$. A concurrent *update* has the following syntax:

switch update	::= `upd(x.fwd(y/z))` | `upd(x.fwd(y/-))` | `upd(x.fwd(-/z))`
sequential update	::= (update `>>` update `>>` ... `>>` update)
parallel update	::= (update `||` update `||` ... `||` update)
update	::= switch update | sequential update | parallel update

where a switch update can renew the forwarding rule of switch `x` from switch `z` to switch `y`, introduce a new forwarding rule from switch `x` to switch `y`, or remove an existing forwarding rule from switch `x` to switch `z`.

4.2 Data Plane and Control Plane as Petri Net with Transits

For a network topology $T = (Sw, Con)$, a set of *ingress* switches, a set of *egress* switches, an initial *forwarding* table, and a concurrent *update*, we show how data and control plane are encoded as Petri net with transits. Switches are modeled by tokens remaining in corresponding places `s` whereas the flow of packets is modeled by the transit relation Υ. Specific transitions $i_{\mathtt{s}}$ model ingress switches where new data flows begin. Tokens in places of the form `x.fwd(y)` configure the forwarding. Data flows are extended by firing transitions `(x,y)` corresponding to configured forwarding without moving any tokens. Thus, we model any order of newly generated packets and their forwarding. Assuming that each existing direction of a connection between two switches is explicitly given in *Con*, we obtain Algorithm 1 which calls Algorithm 2 to obtain the control plane.

input : $T = (Sw, Con)$, *ingress*, *forwarding*, *update*
output: Petri net with transits $\mathcal{N} = (\mathscr{P}, \mathscr{T}, \mathscr{F}, In, \Upsilon)$ for *update* of topology T with *ingress* and *forwarding*

create empty $\mathcal{N} = (\mathscr{P}, \mathscr{T}, \mathscr{F}, In, \Upsilon)$;
for switch `s` $\in Sw$ **do**
  add place `s` to $\mathscr{P}$;
  add place `s` to In;
  if `s` $\in$ *ingress* **then**
    add transition $i_{\mathtt{s}}$ to $\mathscr{T}$;
    add `s` to $pre(i_{\mathtt{s}})$, $post(i_{\mathtt{s}})$;
    add creating data flow $\triangleright\ \Upsilon(i_{\mathtt{s}})$ `s` to Υ;
    add maintaining data flow `s` $\Upsilon(i_{\mathtt{s}})$ `s` to Υ;
for connection `(x,y)` $\in Con$ **do**
  add place `x.fwd(y)` to $\mathscr{P}$;
  if `x.fwd(y)` $\in$ *forwarding* **then**
    add place `x.fwd(y)` to In;
  add transition `(x,y)` to $\mathscr{T}$;
  add `x`, `y`, `x.fwd(y)` to $pre(\mathtt{(x,y)})$, $post(\mathtt{(x,y)})$;
  add connecting data flow `x` Υ`((x,y))` `y` to Υ;
  add maintaining data flow `y` Υ`((x,y))` `y` to Υ;
$\mathcal{N}$ = call Algorithm 2 with T, *update*, $\mathcal{N}$ as input;
add place $update^s$ to In;

Algorithm 1: Data plane

input : $T = (Sw, Con)$, *update*, $\mathcal{N}$
output: $\mathcal{N} = (\mathscr{P}, \mathscr{T}, \mathscr{F}, In, \Upsilon)$
for switch update $u \in SwU$ **do**
  // $u =$ `upd(x.fwd(y/z))`
  add places u^s, u^f to $\mathscr{P}$;
  add transition u to $\mathscr{T}$;
  add u^s to $pre(u)$, u^f to $post(u)$;
  if $z \neq$ `-` **then**
    add `x.fwd(z)` to $pre(u)$;
  if $y \neq$ `-` **then**
    add `x.fwd(y)` to $post(u)$;
for sequential update $s \in SeU$ **do**
  // $s = [s_1, ..., s_i, ..., s_{|s|}]$
  add places s^s, s^f to $\mathscr{P}$;
  for $i \in \{0, ..., |s|\}$ **do**
    add transition s^i to $\mathscr{T}$;
    if $i = 0$ **then**
      add s^s to $pre(s^i)$;
    else
      add s^f_i to $pre(s^i)$;
    if $i = |s|$ **then**
      add s^f to $post(s^i)$;
    else
      add s^s_{i+1} to $post(s^i)$;
for parallel update $p \in PaU$ **do**
  add places p^s, p^f to $\mathscr{P}$;
  add transitions p^o, p^c to $\mathscr{T}$;
  add p^s to $pre(p^o)$, p^f to $post(p^c)$;
  for sub-update u_i of p **do**
    add u^s_i to $post(p^o)$, u^f_i to $pre(p^c)$;

Algorithm 2: Control plane

For the *update*, let SwU be the set of switch updates in it, SeU the set of sequential updates in it, and PaU the set of parallel updates in it. Depending on *update*'s type, it is also added to the respective set. The subnet for the *update* has an empty transit relation but moves tokens from and to places of the form

`x.fwd(y)`. Tokens in these places correspond to the forwarding table. The order of the switch updates is defined by the nesting of sequential and parallel updates. The *update* is realized by a specific token moving through unique places of the form $u^s, u^f, s^s, s^f, p^s, p^f$ for start and finish of each switch update $u \in SwU$, each sequential update $s \in SeU$, and each parallel update $p \in PaU$. A parallel update temporarily increases the number of tokens and reduces it upon completion to one. Algorithm 2 defines the update behavior between start and finish places and connects finish and start places depending on the subexpression structure.

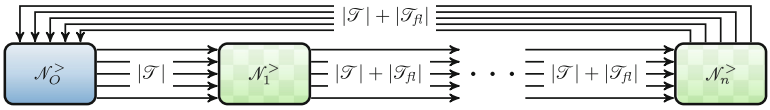

Fig. 3. Overview of the *sequential approach*: Each firing of a transition of the original net is split into first firing a transition in the subnet for the run formula and subsequently firing a transition in each subnet tracking a flow formula. The constructed LTL formula skips the additional steps with until operators.

Fig. 4. Overview of the *parallel approach*: The n subnets are connected such that for every transition $t \in \mathscr{T}$ there are $(|\Upsilon(t)| + 1)^n$ transitions, i.e., there is one transition for every combination of which transit of t (or none) is tracked by which subnet. We use until operators in the constructed LTL formula to only skip steps not involving the tracking of the guessed chain in the flow formula.

4.3 Assumptions and Requirements

We use the run formula $\Diamond\Box \mathit{pre}(t) \rightarrow \Box\Diamond t$ to assume weak fairness for every transition t in our encoding $\mathscr{N}$. Transitions, which are always enabled after some point, are ensured to fire infinitely often. Thus, packets are eventually forwarded and the routing table is eventually updated. We use flow formulas to test specific requirements for all packets. Connectivity ($\mathbb{A}(\Diamond \bigvee_{s \in egress} s)$) ensures that all packets reach an egress switch. Packet coherence ($\mathbb{A}(\Box(\bigvee_{\mathtt{s} \in initial} \mathtt{s}) \vee \Box(\bigvee_{\mathtt{s} \in final} \mathtt{s}))$) tests that packets are either routed according to the initial or final configuration. Drop freedom ($\mathbb{A}\Box(\bigwedge_{\mathtt{e} \in egress} \neg \mathtt{e} \rightarrow \bigvee_{f \in Con} f)$) forbids dropped packets whereas loop freedom ($\mathbb{A}\Box(\bigwedge_{\mathtt{s} \in Sw \setminus egress} \mathtt{s} \rightarrow (\mathtt{s}\ \mathsf{U}\ \Box\neg\mathtt{s}))$) forbids routing loops. We combine run and flow formula into *fairness* $\rightarrow$ *requirement*.

5 Algorithms and Optimizations

Central to model checking a Petri net with transits $\mathcal{N}$ against a Flow-LTL formula φ is the reduction to a safe Petri net $\mathcal{N}^>$ and an LTL formula $\varphi^>$. The infinite state space of the Petri net with transits due to possibly infinitely many flow chains is reduced to a finite state model. The key idea is to guess and track a violating flow chain for each flow subformula $\mathbb{A}\,\psi_i$, for $i \in \{1, \ldots, n\}$, and to only once check the equivalent future of flow chains merging into a common place.

AdamMC provides two approaches for this reduction: Fig. 3 and Fig. 4 give an overview of the *sequential* approach and the *parallel* approach, respectively. Both algorithms create one subnet $\mathcal{N}_i^>$ for each flow subformula $\mathbb{A}\,\psi_i$ to track the corresponding flow chain and have one subnet $\mathcal{N}_O^>$ to check the run part of the formula. The places of $\mathcal{N}_O^>$ are copies of the places in $\mathcal{N}$ such that the current state of the system can be memorized. The subnets $\mathcal{N}_i^>$ also consist of the original places of $\mathcal{N}$ but only use one token (initially residing on an additional place) to track the current state of the considered flow chain. The approaches differ in how these nets are connected to obtain $\mathcal{N}^>$.

Sequential Approach. The places in each subnet $\mathcal{N}_i^>$ are connected with one transition for each transit ($\mathcal{T}_{\not\Pi} = \bigcup_{t \in \mathcal{T}} \Upsilon(t)$). An additional token iterates sequentially through the subnets to activate or deactivate the subnet. This allows each subnet to track a flow chain corresponding to firing a transition in $\mathcal{N}_O^>$. The formula $\varphi^>$ takes care of these additional steps by means of the until operator: In the run part of the formula, all steps corresponding to moves in a subnet $\mathcal{N}_i^>$ are skipped and, for each subformula $\mathbb{A}\,\psi_i$, all steps are skipped until the next transition of the corresponding subnet is fired which transits the tracked flow chain. This technique results in a polynomial increase of the size of the Petri net and the formula: $\mathcal{N}^>$ has $\mathcal{O}(|\mathcal{N}| \cdot n + |\mathcal{N}|)$ places and $\mathcal{O}(|\mathcal{N}|^3 \cdot n + |\mathcal{N}|)$ transitions and the size of $\varphi^>$ is in $\mathcal{O}(|\mathcal{N}|^3 \cdot n \cdot |\varphi| + |\varphi|)$. We refer to [11] for formal details.

Parallel Approach. The n subnets are connected such that the current chain of each subnet is tracked simultaneously while firing an original transition $t \in \mathcal{T}$. Thus, there are $(|\Upsilon(t)|+1)^n$ transitions. Each of these transitions stands for exactly one combination of which subnet is tracking which (or no) transit. Hence, firing one transition of the original net is directly tracked in one step for all subnets. This significantly reduces the complexity of the run part of the constructed formula, since no until operator is needed to skip sequential steps. A disjunction over all transitions corresponding to an original transition suffices to ensure correctness of the construction. Transitions and next operators in the flow parts of the formula still have to be replaced by means of the until operator to ensure that the next step of the tracked flow chain is checked at the corresponding step of the global timeline of $\varphi^>$. In general, the parallel approach results in an exponential blow-up of the net and the formula: $\mathcal{N}^>$ has $\mathcal{O}(|\mathcal{N}| \cdot n + |\mathcal{N}|)$ places and $\mathcal{O}(|\mathcal{N}|^{3n} + |\mathcal{N}|)$ transitions and the size of $\varphi^>$ is in $\mathcal{O}(|\mathcal{N}|^{3n} \cdot |\varphi| + |\varphi|)$. For the practical examples, however, the parallel approach allows for model checking Flow-LTL with few flow subformulas with a tremendous speed-up in comparison to the sequential approach. Formal details are in the full version of the paper [13].

Table 1. Overview of optimization parameters of AdamMC: The three reduction steps depicted in the first column can each be executed by different algorithms. The first step allows to combine the optimizations of the first and second row.

1) Petri Net with Transits $\rightsquigarrow$ Petri Net	sequential		parallel	
	inhibitor	act. token	inhibitor	act. token
2) Petri Net $\rightsquigarrow$ Circuit	explicit		logarithmic	
3) Circuit $\rightsquigarrow$ Circuit	gate optimizations			

Optimizations. Various optimizations parameters can be applied to the model checking routine described in Sect. 3 to tweak the performance. Table 1 gives an overview of the major parameters.

We found that the versions of the sequential and the parallel approach with inhibitor arcs to track flow chains are generally faster than the versions without. Furthermore, the reduction step from a Petri net into a circuit with logarithmically encoded transitions had oftentimes better performance than the same step with explicitly encoded transitions. However, several possibilities to reduce the number of gates of the created circuit worsened the performance of some benchmark families and improved the performance of others. Consequently, all parameters are selectable by the user and a script is provided to compare different settings. An overview of the selectable optimization parameters can be found in the documentation of AdamMC [12]. Our main improvement claims can be retraced by the case study in Sect. 6.

6 Evaluation

We conduct a case study based on SDN with a corresponding artifact [16]. The performance improvements of AdamMC compared to the prototype [10] are summarized in Table 2. For realistic software-defined networks [19], one ingress and one egress switch are chosen at random. Two forwarding tables between the two switches and an update from the first to the second configuration are chosen at random. AdamMC verifies that the update maintained *connectivity* between ingress and egress switch. The results are depicted in rows starting with T. For rows starting with F, we required *connectivity* of a random switch which is not in the forwarding tables. AdamMC falsified this requirement for the update.

The prototype implementation based on an *explicit encoding* can verify updates of networks with 7 switches and falsify updates of networks with 38 switches. We optimize the explicit encoding to a *logarithmic encoding* and the number of switches for which updates can be verified increases to 17. More significantly, the *parallel approach* in combination with the logarithmic encoding leads to tremendous performance gains. The performance gains of an approach with inferior worst-case complexity are mainly due to the smaller complexity of the LTL formula created by the reduction. The encoding of SDN requires fairness assumptions for each transition. These assumptions (encoded in the run

Table 2. We compare the explicit and logarithmic encoding of the sequential approach with the parallel approach. The results are the average over five runs from an Intel i7-2700K CPU with 3.50 GHz, 32 GB RAM, and a timeout (TO) of 30 min. The runtimes are given in seconds.

			expl. enc.			log. enc.			parallel appr.		
T / F	Network	$\#Sw$	Alg.	Time	$\models$	Alg.	Time	$\models$	Alg.	Time	$\models$
T	Arpanet196912	4	IC3	12.08	✓	IC3	9.89	✓	IC3	**2.18**	✓
T	Napnet	6	IC3	146.49	✓	IC3	96.06	✓	IC3	**4.75**	✓
	...			...			...			...	
T	Heanet	7	IC3	806.81	✓	IC3	84.62	✓	IC3	**30.30**	✓
T	HiberniaIreland	7	-	TO	?	-	TO	?	IC3	**26.58**	✓
T	Arpanet19706	9	-	TO	?	IC3	362.21	✓	IC3	**11.33**	✓
T	Nordu2005	9	-	TO	?	-	TO	?	IC3	**12.67**	✓
	...			...			...			...	
T	Fatman	17	-	TO	?	IC3	1543.34	✓	IC3	**162.17**	✓
	...			...			...			...	
T	Myren	37	-	TO	?	-	TO	?	IC3	**1309.23**	✓
T	KentmanJan2011	38	-	TO	?	-	TO	?	IC3	**1261.32**	✓
F	Arpanet196912	4	BMC3	2.18	✗	BMC3	**1.85**	✗	BMC3	1.97	✗
F	Napnet	6	BMC2	4.17	✗	BMC2	5.22	✗	BMC3	**1.48**	✗
	...			...			...			...	
F	Fatman	17	BMC3	168.78	✗	BMC3	169.82	✗	BMC3	**6.72**	✗
	...			...			...			...	
F	Belnet2009	21	BMC2	1146.26	✗	BMC2	611.81	✗	BMC3	**24.26**	✗
	...			...			...			...	
F	KentmanJan2011	38	BMC3	167.92	✗	BMC3	86.44	✗	BMC2	**9.35**	✗
	...			...			...			...	
F	Latnet	69	-	TO	?	-	TO	?	BMC2	**209.20**	✗
F	Ulaknet	82	-	TO	?	-	TO	?	BMC2	**1043.74**	✗
Sum of runtimes (in hours):				82.99			79.15			30.31	
Nb of TOs (of 230 exper.):				146			138			6	

part of the formula) experience a blow-up with until operators by the sequential approach but only need a disjunction in the parallel approach. Hence, the size of networks for which AdamMC can verify updates increases to 38 switches and the size for which it can falsify updates increases to 82 switches. For rather small networks, the tool needs only a few seconds to verify and falsify updates which makes it a great option for operators when updating networks.

7 Related Work

We refer to [21] for an introduction to SDN. Solutions for correctness of updates of software-defined networks include *consistent updates* [7,28], *dynamic scheduling* [17], and *incremental updates* [18]. Both explicit and SMT-based model checking [1,5,22,23,26,31] is used to verify software-defined networks. Closest to our approach are models of networks as Kripke structures to use model checking

for synthesis of correct network updates [8,24]. The model checking subroutine of the synthesizer assumes that each packet sees at most one updated switch. Our model checking routine does not make such an assumption.

There is a significant number of model checking tools (e.g., [29,32]) for Petri nets and an annual model checking contest [20]. AdamMC is restricted to safe Petri nets whereas other tools can handle bounded and colored Petri nets. At the same time, only AdamMC accepts LTL formulas with places *and* transitions as atomic propositions. This is essential to express fairness in our SDN encoding.

8 Conclusion

We presented the tool AdamMC with its three application domains: checking safe Petri nets with transits against Flow-LTL, checking concurrent updates of software-defined networks against common assumptions and specifications, and checking safe Petri nets against LTL. New algorithms allow AdamMC to model check software-defined networks of realistic size: it can verify updates of networks with up to 38 switches and can falsify updates of networks with up to 82 switches.

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Action-Based Model Checking: Logic, Automata, and Reduction

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Abstract. Stutter invariant properties play a special role in state-based model checking: they are the properties that can be checked using partial order reduction (POR), an indispensable optimization. There are algorithms to decide whether an LTL formula or Büchi automaton (BA) specifies a stutter-invariant property, and to convert such a BA to a form that is appropriate for on-the-fly POR-based model checking.

The *interruptible* properties play the same role in action-based model checking that stutter-invariant properties play in the state-based case. These are the properties that are invariant under the insertion or deletion of "invisible" actions. We present algorithms to decide whether an LTL formula or BA specifies an interruptible property, and show how a BA can be transformed to an *interrupt normal form* that can be used in an on-the-fly POR algorithm. We have implemented these algorithms in a new model checker named McRERS, and demonstrate their effectiveness using the RERS 2019 benchmark suite.

Keywords: Model checking · Action · Event · LTL · Stutter-invariant

1 Introduction

To apply model checking to a concurrent system, one must formulate properties that the system is expected to satisfy. A property may be expressed by specifying acceptable sequences of states, or by specifying acceptable sequences of actions—the events that cause the state to change. Each approach has advantages and disadvantages, and in any particular context one may be more appropriate than the other.

In the state-based context, there is a rich theory involving automata, logic, and reduction for model checking. Some of the core ideas in this theory can be summarized as follows. First, the behavior of the concurrent system is represented by a state-transition system T. One identifies a set AP of atomic propositions, and each state of T is labeled by the set of propositions which hold at that state. An execution passes through an infinite sequence of states, which defines a *trace*, i.e., a sequence of subsets of AP. A *property* is a set of traces, and T satisfies the property if every trace of T is in P.

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Properties may be specified by formulas in a temporal logic, such as LTL [26]. There are algorithms (e.g., [37]) to convert an LTL formula ϕ to an equivalent Büchi automaton (BA) B_ϕ with alphabet 2^{AP}. (Properties may also be specified directly using BAs.) The system T satisfies ϕ if and only if the language of the synchronous product $T \otimes B_{\neg\phi}$ is empty. The emptiness of the language can be determined on-the-fly, i.e., while the reachable states of the product are being constructed.

A property P is *stutter-invariant* if it is closed under the insertion and deletion of repetitions, i.e., $s_0 s_1 \cdots \in P \;\Leftrightarrow\; s_0^{i_0} s_1^{i_1} \cdots \in P$ holds for any positive integers $i_0, i_1, \cdots$. Many algorithms are known for deciding whether an LTL formula or a BA specifies a stutter-invariant property [22,24]. There is also an argument that only stutter-invariant properties should be used in practice. For example, suppose that a trace is formed by sampling the state of a system once every millisecond. If we sample the same system twice each millisecond, and there are no state changes in the sub-millisecond intervals, the second trace will be stutter-equivalent to the first. A meaningful property should be invariant under this choice of time resolution.

Stutter-invariant properties are desirable for another reason: they admit the most significant optimization in model checking, partial order reduction (POR, [15,23,25]). At each state encountered in the exploration of the product space, an on-the-fly POR scheme produces a subset of the enabled transitions. Restricting the search to the transitions in those subsets does not affect the language emptiness question. Recent work has revealed that the BA must have a certain form—"SI normal form"—when POR is used with on-the-fly model checking, but any BA with a stutter-invariant language can be easily transformed into SI normal form [27].

The purpose of this paper is to elaborate an analogous theory for event-based models. Event-based models of concurrency are widely used and have been extremely influential for over three decades. For example, process algebras, such as CSP, are event-based and use *labeled transition systems* (LTSs) for the semantic model. Event-based models are the main formalism used in assume-guarantee reasoning (e.g, [10]), and in many other areas. There are mature model checking and verification tools for process algebras and LTSs, and which have significant industrial applications; see, e.g., [13]. Temporal logics, including LTL, CTL, and CTL*, have long been used to specify event-based systems [3,7,12].

We call the class of properties in the action context that are analogous to the stutter-invariant properties in the state context the *interruptible* properties (Sect. 3). These properties are invariant under "action stuttering" [34], i.e., the insertion or deletion of "invisible" actions. We present algorithms for deciding whether an LTL formula or a BA specifies an interruptible property (Theorems 1 and 2); to the best of our knowledge, these are the first published algorithms for deciding this property of formulas or automata.

Interruptible properties play the same role in action-based POR that stutter-invariant properties play in state-based POR. In particular, we present an action-based on-the-fly POR algorithm that works for interruptible properties (Sect. 4).

As with the state-based case, the algorithm requires that the BA be in a certain normal form. We introduce a novel *interrupt normal form* (Definition 11) for this purpose, and show how any BA with an interruptible language can be transformed into that form. The relation to earlier work is discussed in Sect. 5. The effectiveness of these reduction techniques is demonstrated by applying them to problems in the 2019 RERS benchmark suite (Sect. 6).

2 Preliminaries

Let S be a set. 2^S denotes the set of all subsets of S. S^* denotes the set of finite sequences of elements of S; S^ω the infinite sequences. Let $\zeta = s_0 s_1 \cdots$ be a (finite or infinite) sequence and $i \geq 0$. If ζ is finite of length n, assume $i < n$. Then $\zeta(i)$ denotes the element s_i. For any $i \geq 0$, ζ^i denotes the suffix $s_i s_{i+1} \cdots$. (ζ^i is empty if ζ is finite and $i \geq n$).

For $\zeta \in S^*$ and $\eta \in S^* \cup S^\omega$, $\zeta \circ \eta$ denotes the concatenation of ζ and η.

If $S \subseteq T$ and η is a sequence of elements of T, $\eta|_S$ denotes the sequence obtained by deleting from η all elements not in S.

2.1 Linear Temporal Logic

Let Act be a universal set of actions. We assume Act is infinite.

Definition 1. Form (the *LTL formulas over* Act) is the smallest set satisfying:

- $\mathsf{true} \in \mathsf{Form}$,
- if $a \in \mathsf{Act}$ then $a \in \mathsf{Form}$, and
- if f and g are in Form, so are $\neg f$, $f \wedge g$, $\mathbf{X}f$, and $f\mathbf{U}g$.

Additional operators are defined as shorthand for other formulas: $\mathsf{false} = \neg\mathsf{true}$, $f \vee g = \neg((\neg f) \wedge \neg g)$, $f \rightarrow g = (\neg f) \vee g$, $\mathbf{F}f = \mathsf{true}\mathbf{U}f$, $\mathbf{G}f = \neg\mathbf{F}\neg f$, and $f\mathbf{W}g = (f\mathbf{U}g) \vee \mathbf{G}f$. □

Definition 2. The *alphabet* of an LTL formula f, denoted αf, is the set of actions that occur syntactically within f. □

Definition 3. The *action-based semantics* of LTL is defined by the relation $\zeta \models_A f$, where $\zeta \in \mathsf{Act}^\omega$ and $f \in \mathsf{Form}$, which is defined as follows:

- $\zeta \models_A \mathsf{true}$,
- $\zeta \models_A a$ iff $\zeta(0) = a$,
- $\zeta \models_A \neg f$ iff $\zeta \not\models_A f$,
- $\zeta \models_A f \wedge g$ iff $\zeta \models_A f$ and $\zeta \models_A g$,
- $\zeta \models_A \mathbf{X}f$ iff $\zeta^1 \models_A f$, and
- $\zeta \models_A f\mathbf{U}g$ iff $\exists i \geq 0 \,.\, (\zeta^i \models_A g \wedge \forall j \in 0..i-1 \,.\, \zeta^j \models_A f)$. □

When using the action-based semantics, the logic is sometimes referred to as "Action LTL" or ALTL [11,12].

The *state-based semantics* is defined by a relation $\xi \models_{\mathsf{S}} f$, where $\xi \in (2^{\mathsf{Act}})^\omega$. The definition of $\models_{\mathsf{S}}$ is well-known, and is exactly the same as Definition 3, except that $\xi \models_{\mathsf{S}} a$ iff $a \in \xi(0)$. The action semantics are consistent with the state semantics in the following sense. Let $f \in \mathsf{Form}$, and $\zeta = a_0 a_1 \cdots \in \mathsf{Act}^\omega$. Let $\xi = \{a_0\}\{a_1\}\cdots \in (2^{\mathsf{Act}})^\omega$. Then $\zeta \models_{\mathsf{A}} f$ iff $\xi \models_{\mathsf{S}} f$. The main difference between the state- and action-based formalisms is that in the state-based formalism, any number of atomic propositions can hold at each step. In the action-based formalism, precisely one action occurs in each step.

Definition 4. Let $f, g \in \mathsf{Form}$. Define

- (action equivalence) $f \equiv_{\mathsf{A}} g$ if $(\zeta \models_{\mathsf{A}} f \Leftrightarrow \zeta \models_{\mathsf{A}} g)$ for all $\zeta \in \mathsf{Act}^\omega$
- (state equivalence) $f \equiv_{\mathsf{S}} g$ if $(\xi \models_{\mathsf{S}} f \Leftrightarrow \xi \models_{\mathsf{S}} g)$ for all $\xi \in (2^{\mathsf{Act}})^\omega$. □

The following fact about the state-based semantics can be proved by induction on the formula structure:

Lemma 1. *Let $f \in \mathsf{Form}$ and $\xi = s_0 s_1 \cdots \in (2^{\mathsf{Act}})^\omega$. Let $\xi' = s'_0 s'_1 \cdots$, where $s'_i = \alpha f \cap s_i$. Then $\xi \models_{\mathsf{S}} f$ iff $\xi' \models_{\mathsf{S}} f$.*

The following shows that action LTL, like ordinary state-based LTL, is a decidable logic:

Proposition 1. *Let $f, g \in \mathsf{Form}$, $A = \alpha f \cup \alpha g$, and*

$$h = \mathbf{G}\Big[\Big(\bigwedge_{a\in A} \neg a\Big) \vee \bigvee_{a\in A} \Big(a \wedge \bigwedge_{b\in A\setminus\{a\}} \neg b\Big)\Big].$$

Then $f \equiv_{\mathsf{A}} g \Leftrightarrow f \wedge h \equiv_{\mathsf{S}} g \wedge h$. In particular, action equivalence is decidable.

Proof. Note the meaning of h: at each step in a state-based trace, at most one element of A is true.

Suppose $f \wedge h \equiv_{\mathsf{S}} g \wedge h$. Let $\zeta = a_0 a_1 \cdots \in \mathsf{Act}^\omega$. Let $\xi = \{a_0\}\{a_1\}\cdots$. We have $\xi \models_{\mathsf{S}} h$. By the consistency of the state and action semantics, we have

$$\zeta \models_{\mathsf{A}} f \Leftrightarrow \xi \models_{\mathsf{S}} f \Leftrightarrow \xi \models_{\mathsf{S}} f \wedge h \Leftrightarrow \xi \models_{\mathsf{S}} g \wedge h \Leftrightarrow \xi \models_{\mathsf{S}} g \Leftrightarrow \zeta \models_{\mathsf{A}} g,$$

hence $f \equiv_{\mathsf{A}} g$.

Suppose instead that $f \equiv_{\mathsf{A}} g$. We wish to show $\xi \models_{\mathsf{S}} f \wedge h \Leftrightarrow \xi \models_{\mathsf{S}} g \wedge h$ for any $\xi = s_0 s_1 \cdots \in (2^{\mathsf{Act}})^\omega$. By Lemma 1, it suffices to assume $s_i \subseteq A$ for all i.

Let τ be any element of $\mathsf{Act} \setminus A$. (Here we are using the fact that Act is infinite, while A is finite.) If $|s_i| > 1$ for some i, then ξ violates h and therefore violates both $f \wedge h$ and $g \wedge h$. So suppose $|s_i| \leq 1$ for all i, which means $\xi \models_{\mathsf{S}} h$. Let $\zeta = a_0 a_1 \cdots$, where a_i is the sole member of s_i if $|s_i| = 1$, or τ if $|s_i| = 0$. By Lemma 1, $\xi \models_{\mathsf{S}} f$ iff $\{a_0\}\{a_1\}\cdots \models_{\mathsf{S}} f$. By the consistency of the action and state semantics, this is equivalent to $\zeta \models_{\mathsf{A}} f$. A similar statement holds for g. Hence

$$\xi \models_{\mathsf{S}} f \wedge h \Leftrightarrow \xi \models_{\mathsf{S}} f \Leftrightarrow \zeta \models_{\mathsf{A}} f \Leftrightarrow \zeta \models_{\mathsf{A}} g \Leftrightarrow \xi \models_{\mathsf{S}} g \Leftrightarrow \xi \models_{\mathsf{S}} g \wedge h.$$

The proposition reduces the question of action equivalence to one of ordinary (state) equivalence of LTL formulas, which is known to be decidable ([26], see also [36, Thm. 24]). □

Definition 5. For $A \subseteq \mathsf{Act}$ and $f \in \mathsf{Form}$ with $\alpha f \subseteq A$, let

$$\mathcal{L}(f, A) = \{\zeta \in A^\omega \mid \zeta \models f\}.$$

□

2.2 Büchi Automata

Definition 6. A *Büchi Automaton* (BA) over Act is a tuple $(S, \Sigma, \rightarrow, S^0, F)$ where

1. S is a finite set of *states*,
2. Σ, the *alphabet*, is a finite subset of Act,
3. $\rightarrow \subseteq S \times \Sigma \times S$ is the *transition relation*,
4. $S^0 \subseteq S$ is the set of *initial states*, and
5. $F \subseteq S$ is the set of *accepting states*. □

We will use the following notation and terminology for a BA B. The *source* of a transition (s, a, s') is s, the *destination* is s', and the *label* is a. We write $s \xrightarrow{a} s'$ as shorthand for $(s, a, s') \in \rightarrow$, and $s \xrightarrow{a_0 a_1 \ldots a_n} s'$ for $\exists s_1, s_2, \ldots s_n \in S \,.\, s \xrightarrow{a_0} s_1 \xrightarrow{a_1} s_2 \ldots s_n \xrightarrow{a_n} s'$. For $a \in A$ and $s \in S$, we say a is *enabled at* s if $s \xrightarrow{a} s'$ for some $s' \in S$. The set of all actions enabled at s is denoted $\mathsf{enabled}(B, s)$.

For $s \in S$, a *path in* B *starting from* s is a (finite or infinite) sequence π of transitions such that (1) if π is not empty, the source of $\pi(0)$ is s, and (2) the destination of $\pi(i)$ is the source of $\pi(i+1)$ for all i for which these are defined. If π is not empty, define $\mathsf{first}(\pi)$ to be s; if π is finite, define $\mathsf{last}(\pi)$ to be the destination of the last transition of π. We say π *spells the word* $a_0 a_1 \cdots$, where a_i is the label of $\pi(i)$.

An infinite path is *accepting* if it visits a state in F infinitely often. An *(accepting) trace starting from* s is a word spelled by an (accepting) path starting from s. An *(accepting) trace of* B is an (accepting) trace starting from an initial state. The *language of* B, denoted $\mathcal{L}(B)$, is the set of all accepting traces of B.

Proposition 2. *There is an algorithm that consumes any finite subset* A *of* Act *and an* $f \in \mathsf{Form}$ *with* $\alpha f \subseteq A$*, and produces a BA* B *with alphabet* A *such that* $\mathcal{L}(B) = \mathcal{L}(f, A)$*.*

Proof. There are well-known algorithms to produce a BA C with alphabet 2^A which accepts exactly the words satisfying f under the state semantics (e.g., [37]). Let B be the same as C, except the alphabet is A and there is a transition $s \xrightarrow{a} s'$ in B iff there is a transition $s \xrightarrow{\{a\}} s'$ in C. We have

$$\begin{aligned} a_0 a_1 \cdots \in \mathcal{L}(B) &\Leftrightarrow \{a_0\}\{a_1\} \cdots \in \mathcal{L}(C) \\ &\Leftrightarrow \{a_0\}\{a_1\} \cdots \models_{\mathsf{s}} f \\ &\Leftrightarrow a_0 a_1 \cdots \in \mathcal{L}(f, A). \end{aligned}$$

□

In practice, tools that convert LTL formulas to BAs produce an automaton in which an edge is labeled by a propositional formula ϕ over αf. Such an edge represents a set of transitions, one for each $P \subseteq A$ for which ϕ holds for the valuation that assigns *true* to each element of P and *false* to each element of $A \setminus P$. In this case, the conversion to B entails creating one transition for each $a \in A$ for which ϕ holds when *true* is assigned to a and *false* is assigned to all other actions.

Definition 7. Let $B_i = (S_i, \Sigma_i, \rightarrow_i, S_i^0, F_i)$ $(i = 1, 2)$ denote two BAs over Act. The *parallel composition of* B_1 *and* B_2 is the BA

$$B_1 \parallel B_2 \equiv (S_1 \times S_2, \Sigma_1 \cup \Sigma_2, \rightarrow, S_1^0 \times S_2^0, F_1 \times F_2),$$

where $\rightarrow$ is defined by

$$\frac{s_1 \xrightarrow{a}_1 s_1' \quad a \notin \Sigma_2}{\langle s_1, s_2\rangle \xrightarrow{a} \langle s_1', s_2\rangle} \qquad \frac{s_2 \xrightarrow{a}_2 s_2' \quad a \notin \Sigma_1}{\langle s_1, s_2\rangle \xrightarrow{a} \langle s_1, s_2'\rangle} \qquad \frac{s_1 \xrightarrow{a}_1 s_1' \quad s_2 \xrightarrow{a}_2 s_2'}{\langle s_1, s_2\rangle \xrightarrow{a} \langle s_1', s_2'\rangle}.$$

□

If we flatten all tuples (e.g., identify $(S_1 \times S_2) \times S_3$ with $S_1 \times S_2 \times S_3$) then $\parallel$ is an associative operator.

Note that in the special case where the two automata have the same alphabet ($\Sigma_1 = \Sigma_2$), every action is synchronizing, and the parallel composition is the usual "synchronous product." In this case, $\mathcal{L}(B_1 \parallel B_2) = \mathcal{L}(B_1) \cap \mathcal{L}(B_2)$.

2.3 Labeled Transition Systems

Definition 8. A *labeled transition system* (LTS) over Act is a tuple $(Q, A, \rightarrow, q^0)$ for which $(Q, A, \rightarrow, \{q^0\}, Q)$ is a BA over Act. In other words, it is a BA in which all states are accepting and there is only one initial state. □

Definition 9. Let M be an LTS with alphabet A, and f an LTL formula with $\alpha f \subseteq A$. We write $M \models f$ if $\mathcal{L}(M) \subseteq \mathcal{L}(f, A)$. □

The following observation is the basis of the automata-theoretic approach to model checking (cf. [36, §4.2]):

Proposition 3. *Let M be an LTS with alphabet A and f an LTL formula with $\alpha f \subseteq A$. Let B be a BA with $\mathcal{L}(B) = \mathcal{L}(\neg f, A)$. Then $M \models f \Leftrightarrow \mathcal{L}(M \parallel B) = \emptyset$.*

Proof. M and B have the same alphabet, so $\mathcal{L}(M \parallel B) = \mathcal{L}(M) \cap \mathcal{L}(B)$, hence

$$\mathcal{L}(M \parallel B) = \mathcal{L}(M) \cap \mathcal{L}(\neg f, A) = \mathcal{L}(M) \cap (A^\omega \setminus \mathcal{L}(f, A)) = \mathcal{L}(M) \setminus \mathcal{L}(f, A).$$

This set is empty iff $\mathcal{L}(M) \subseteq \mathcal{L}(f, A)$. □

There are various algorithms to determine language emptiness of a BA; in this paper we use the well-known Nested Depth First Search (NDFS) algorithm [2].

3 Interruptible Properties

3.1 Definition and Examples

An LTS comes with an alphabet, which is a subset A of Act. By a *property over* A we simply mean a subset P of A^ω. We say a trace $\zeta \in A^\omega$ *satisfies* P if $\zeta \in P$. We have already seen two ways to specify properties. An LTL formula f with $\alpha f \subseteq A$ specifies the property $\mathcal{L}(f, A)$. A Büchi automaton B with alphabet A specifies the property $\mathcal{L}(B)$. We next define a special class of properties:

Definition 10. Given sets $V \subseteq A \subseteq \mathsf{Act}$, we say a property P over A is *V-interruptible* if

$$\zeta|_V = \eta|_V \Rightarrow (\zeta \in P \;\Leftrightarrow\; \eta \in P) \qquad \text{for all } \zeta, \eta \in A^\omega.$$

An LTL formula f is *V-interruptible* if $\mathcal{L}(f, \mathsf{Act})$ is V-interruptible. We say f is *interruptible* if f is αf-interruptible. The set of all interruptible LTL formulas is denoted Intrpt. □

The set V is known as the *visible set*. The definition essentially says that the insertion or deletion of invisible actions (those in $A \backslash V$) has no bearing on whether a trace satisfies P. Put another way, the question of whether a trace belongs to P is determined purely by its visible actions. The following collects some basic facts about interruptibility. All follow immediately from the definitions.

Proposition 4. *Let $V \subseteq A \subseteq \mathsf{Act}$, $P \subseteq A^\omega$ and $f, g \in \mathsf{Form}$. Then all of the following hold:*

1. *P is A-interruptible.*
2. *If P is V-interruptible, and $V \subseteq V'$, then P is V'-interruptible.*
3. *If f is interruptible and $\alpha f \subseteq A$, then $\mathcal{L}(f, A)$ is αf-interruptible.*
4. *f is interruptible iff the following holds:*

$$\forall \zeta, \eta \in \mathsf{Act}^\omega \,.\, (\zeta|_{\alpha f} = \eta|_{\alpha f} \wedge \zeta \;\models_{\mathsf{A}}\; f) \Rightarrow \eta \;\models_{\mathsf{A}}\; f.$$

5. *If $\alpha f = \alpha g$ and $f \equiv_{\mathsf{A}} g$ then f is interruptible iff g is interruptible.*

Many, if not most, properties that arise in practice are V-interruptible for the set V of actions that are mentioned in the property. Assuming a, b, and c are distinct actions, we have:

- For any $n \geq 0$, the property "a occurs at most n times" is $\{a\}$-interruptible, since the insertion or deletion of actions other than a cannot affect whether a word satisfies that property. The same is true for the properties "a occurs at least n times" and "a occurs exactly n times." These are examples of the *bounded existence pattern with global scope* in a widely used property specification pattern system [5]. LTL formulas in this category include $\mathbf{G}\neg a$ (a occurs 0 times), $\mathbf{F}a$ (a occurs at least once), and $\mathbf{F}(a \wedge \mathbf{XF}a)$ (a occurs at least twice).

- The property "after any occurrence of a, b eventually occurs", $\mathbf{G}(a \to \mathbf{F}b)$, is $\{a, b\}$-interruptible. This is the *response pattern with global scope* [5].
- The property "after any occurrence of a, c will eventually occur, and no b will occur until c", $\mathbf{G}(a \to ((\neg b)\mathbf{U}c))$, is $\{a, b, c\}$-interruptible. This is a variation on the *absence pattern with after-until scope*, and is used to specify mutual exclusion [5].

On the other hand, the property "a occurs at time 0", (LTL formula a) is not $\{a\}$-interruptible. Neither is "an event other than a occurs at least once" ($\mathbf{F}\neg a$) nor "only a occurs" ($\mathbf{G}a$). The property "every occurrence of a is followed immediately by b," formula $\mathbf{G}(a \to \mathbf{X}b)$, is not $\{a, b\}$-interruptible. The property "after any occurrence of a, c eventually occurs and until then only b occurs," $\mathbf{G}(a \to \mathbf{X}(b\mathbf{U}c))$, is not $\{a, b, c\}$-interruptible.

The following provides a useful way to show that two interruptible properties are equal:

Lemma 2. *Suppose $V \subseteq A \subseteq \mathsf{Act}$ and P_1 and P_2 are V-interruptible properties over A. Let $\mathcal{F} = V^\omega \cup V^* \circ (A \setminus V)^\omega$. Then $P_1 = P_2$ iff $P_1 \cap \mathcal{F} = P_2 \cap \mathcal{F}$.*

Proof. Assume $P_1 \cap \mathcal{F} = P_2 \cap \mathcal{F}$. Let $\zeta \in P_1$. If $\zeta|_V$ is infinite, then since $\zeta|_V|_V = \zeta|_V$, and P_1 is V-interruptible, $\zeta|_V \in P_1$. But $\zeta|_V \in V^\omega$, so $\zeta|_V \in P_1 \cap \mathcal{F}$, and therefore $\zeta|_V \in P_2$. Since P_2 is V-interruptible, $\zeta \in P_2$.

If $\zeta|_V$ is finite, there is a prefix θ of ζ such that $\zeta = \theta \circ \eta$, with $\eta \in (V \setminus A)^\omega$. Let $\xi = \theta|_V \circ \eta$. We have $\xi \in V^* \circ (A \setminus V)^\omega$ and $\xi|_V = \zeta|_V$, hence $\xi \in P_1 \cap \mathcal{F}$. Therefore $\xi \in P_2$, and since P_2 is V-interruptible, $\zeta \in P_2$. □

The elements of $\mathcal{F}$ are known as the *V-interrupt-free* words over A.

3.2 Decidability of Interruptibility of LTL Formulas

We next show that interruptibility is a decidable property of LTL formulas. Define $\mathsf{intrpt}\colon \mathsf{Form} \to \mathsf{Form}$ as follows. Given $f \in \mathsf{Form}$, let $V = \alpha f$ and $\hat{V} = \bigvee_{a \in V} a$, and define $\beta\colon \mathsf{Form} \to \mathsf{Form}$ by

$$\begin{aligned}
\beta(\mathsf{true}) &= \mathsf{true} \\
\beta(a) &= (\neg\hat{V})\mathbf{U}a \\
\beta(\neg f_1) &= \neg\beta(f_1) \\
\beta(f_1 \wedge f_2) &= \beta(f_1) \wedge \beta(f_2) \\
\beta(\mathbf{X}f_1) &= ((\neg\hat{V})\mathbf{U}(\hat{V} \wedge \mathbf{X}\beta(f_1))) \vee ((\mathbf{G}\neg\hat{V}) \wedge \mathbf{X}\beta(f_1)) \\
\beta(f_1\mathbf{U}f_2) &= \beta(f_1)\mathbf{U}\beta(f_2).
\end{aligned}$$

for $a \in \mathsf{Act}$ and $f_1, f_2 \in \mathsf{Form}$. Let $\mathsf{intrpt}(f) = \beta(f)$.

Theorem 1. *Let f be an LTL formula over Act. The following hold:*

1. *$\mathsf{intrpt}(f)$ is interruptible.*
2. *f is interruptible iff $\mathsf{intrpt}(f) \equiv_{\mathsf{A}} f$.*

In particular, interruptibility of LTL formulas is decidable.

Before proving Theorem 1, we give some intuition regarding the definition of intrpt. Function β can be thought of as consuming a property on V-interrupt-free words (i.e., words in $V^\omega \cup V^* \circ (A \setminus V)^\omega$) and extending it to a property on all words (A^ω). It is designed so that $\beta(g)$ is V-interruptible and agrees with g on V-interrupt-free words. For example, the formula a means "a is the first action" (in an interrupt-free word), which extends to the property "a is the first visible action" (in an arbitrary word). The formula $\mathbf{X}f_1$ states "f_1 holds after removing the first action," so $\beta(\mathbf{X}f_1)$ should declare "$\beta(f_1)$ holds after removing the prefix ending in the first visible action." That is almost correct, but there is also the possibility that an element of A^ω has no visible action, which is the reason for the second clause in the definition of $\beta(\mathbf{X}f_1)$.

The remainder of this subsection is devoted to the proof of Theorem 1. First note that $\mathsf{intrpt}(f)$ and f have the same alphabet, i.e., $\alpha\mathsf{intrpt}(f) = V$.

Proof of Part 1. Say a subformula g of f is *good* if $\beta(g)$ is V-interruptible, i.e.,

$$\forall \zeta, \eta \in \mathsf{Act}^\omega \,.\, \zeta|_V = \eta|_V \Rightarrow (\zeta \models_{\mathsf{A}} \beta(g) \Leftrightarrow \eta \models_{\mathsf{A}} \beta(g)).$$

We show by induction on formula structure that every subformula of f is good. The case $g = f$ will show that $\mathsf{intrpt}(f)$ is interruptible. Assume throughout that $\zeta|_V = \eta|_V$.

If $g = \mathsf{true}$ then $\beta(g) = \mathsf{true}$, so g is clearly good.

If $g = a$ for some $a \in \mathsf{Act}$, then $\zeta \models_{\mathsf{A}} \beta(g) = (\neg\hat{V})\mathbf{U}a$ iff $\zeta|_V$ is non-empty and $\zeta|_V(0) = a$. Since this depends only on $\zeta|_V$, g is good.

If $g = \neg f_1$ and f_1 is good, then g is good because

$$\zeta \models_{\mathsf{A}} \beta(g) \Leftrightarrow \zeta \not\models_{\mathsf{A}} \beta(f_1) \Leftrightarrow \eta \not\models \beta(f_1) \Leftrightarrow \eta \models_{\mathsf{A}} \beta(g).$$

If $g = f_1 \wedge f_2$, and f_1 and f_2 are good, then g is good because

$$\begin{aligned} \zeta \models_{\mathsf{A}} \beta(g) &\Leftrightarrow \zeta \models_{\mathsf{A}} \beta(f_1) \wedge \zeta \models_{\mathsf{A}} \beta(f_2) \\ &\Leftrightarrow \eta \models_{\mathsf{A}} \beta(f_1) \wedge \eta \models_{\mathsf{A}} \beta(f_2) \Leftrightarrow \eta \models_{\mathsf{A}} \beta(g). \end{aligned}$$

Suppose $g = \mathbf{X}f_1$ and f_1 is good. There are two cases:

- **Case 1:** $\zeta|_V$ is empty. Then no suffix of ζ or η satisfies $\hat{V}$. Hence

$$\theta \models_{\mathsf{A}} \beta(g) \Leftrightarrow \theta \models_{\mathsf{A}} \mathbf{X}\beta(f_1) \Leftrightarrow \theta^1 \models_{\mathsf{A}} \beta(f_1) \qquad (\theta \in \{\zeta, \eta\}).$$

  Moreover, $\zeta^1|_V = \eta^1|_V$ (as both are empty), and $\beta(f_1)$ is good, so we have $\zeta^1 \models_{\mathsf{A}} \beta(f_1) \Leftrightarrow \eta^1 \models_{\mathsf{A}} \beta(f_1)$. These show $\zeta \models_{\mathsf{A}} \beta(g) \Leftrightarrow \eta \models_{\mathsf{A}} \beta(g)$.
- **Case 2:** $\zeta|_V$ is nonempty. Let i be the index of the first occurrence of an element of V in ζ, and j the similar index for η. We have

$$\zeta^{i+1}|_V = (\zeta|_V)^1 = (\eta|_V)^1 = \eta^{j+1}|_V.$$

  As f_1 is good, it follows that $\zeta^{i+1} \models_{\mathsf{A}} \beta(f_1) \Leftrightarrow \eta^{j+1} \models_{\mathsf{A}} \beta(f_1)$. Hence

$$\zeta \models_{\mathsf{A}} \beta(g) \Leftrightarrow \zeta^{i+1} \models_{\mathsf{A}} \beta(f_1) \Leftrightarrow \eta^{j+1} \models_{\mathsf{A}} \beta(f_1) \Leftrightarrow \eta \models_{\mathsf{A}} \beta(g).$$

Suppose $g = f_1 \mathbf{U} f_2$ and f_1 and f_2 are good. We have $\beta(g) = \beta(f_1)\mathbf{U}\beta(f_2)$. If $\zeta \models_A \beta(g)$ then there exists $i \geq 0$ such that $\zeta^i \models_A \beta(f_2)$ and $\zeta^j \models_A \beta(f_1)$ for $j < i$. Now there is some $i' \geq 0$ such that $\eta^{i'}|_V = \zeta^i|_V$ and for all $j' < i'$, there is some $j < i$ such that $\eta^{j'}|_V = \zeta^j|_V$. It follows that $\eta \models \beta(g)$. Hence g is good.

Proof of Part 2. Suppose first that $\mathsf{intrpt}(f) \equiv_A f$. From part 1, $\mathsf{intrpt}(f)$ is interruptible, so Proposition 4(5) implies f is interruptible.

Suppose instead that f is interruptible. We wish to show $\mathsf{intrpt}(f) \equiv_A f$. By Lemma 2, it suffices to show the two formulas agree on V-interrupt-free words. We will show by induction that for each subformula g of f, $\zeta \models_A g \Leftrightarrow \zeta \models_A \beta(g)$ for all V-interrupt-free ζ. The case $g = f$ will complete the proof.

If $g = \mathsf{true}$, $\beta(g) = \mathsf{true}$ and the condition clearly holds.

If $g = a$ for some $a \in \mathsf{Act}$, $\zeta \models_A \beta(g) \Leftrightarrow \zeta \models_A (\neg\hat{V})\mathbf{U}a \Leftrightarrow \zeta \models_A a$, as ζ is V-interrupt-free.

If $g = \neg f_1$ and the inductive hypothesis holds for f_1, then

$$\zeta \models_A \beta(g) \Leftrightarrow \zeta \not\models_A \beta(f_1) \Leftrightarrow \zeta \not\models_A f_1 \Leftrightarrow \zeta \models_A g.$$

If $g = f_1 \wedge f_2$ and the inductive hypothesis holds for f_1 and f_2 then

$$\zeta \models_A \beta(g) \Leftrightarrow \zeta \models_A \beta(f_1) \wedge \zeta \models_A \beta(f_2) \Leftrightarrow \zeta \models_A f_1 \wedge \zeta \models_A f_2 \Leftrightarrow \zeta \models_A g.$$

Suppose $g = \mathbf{X} f_1$ and the inductive hypothesis holds for f_1. Note that any suffix of a V-interrupt-free word, e.g., ζ^1, is also V-interrupt-free. If $\zeta|_V$ is empty,

$$\zeta \models_A \beta(g) \Leftrightarrow \zeta \models_A \mathbf{X}\beta(f_1) \Leftrightarrow \zeta^1 \models_A \beta(f_1) \Leftrightarrow \zeta^1 \models_A f_1 \Leftrightarrow \zeta \models_A g.$$

If $\zeta|_V$ is nonempty, then $\zeta \models_A \hat{V}$, so

$$\begin{aligned} \zeta \models_A \beta(g) &\Leftrightarrow \zeta \models_A (\neg\hat{V})\mathbf{U}(\hat{V} \wedge \mathbf{X}\beta(f_1)) \Leftrightarrow \zeta \models_A \mathbf{X}\beta(f_1) \\ &\Leftrightarrow \zeta^1 \models_A \beta(f_1) \Leftrightarrow \zeta^1 \models_A f_1 \Leftrightarrow \zeta \models_A g. \end{aligned}$$

If $g = f_1 \mathbf{U} f_2$, then applying the inductive hypothesis to f_1 and f_2 yields

$$\begin{aligned} \zeta \models_A g &\Leftrightarrow \exists i > 0 \,.\, \zeta^i \models_A f_2 \wedge \forall j < i \,.\, \zeta^j \models_A f_1 \\ &\Leftrightarrow \exists i > 0 \,.\, \zeta^i \models_A \beta(f_2) \wedge \forall j < i \,.\, \zeta^j \models_A \beta(f_1) \\ &\Leftrightarrow \zeta \models_A \beta(g). \end{aligned}$$

Decidability follows from part 2 and Proposition 1. This completes the proof of Theorem 1.

Remark 1. The definition of $\beta(\mathbf{X} f_1)$ is convenient for the proof but shorter definitions also work. If the formula f_1 is satisfied by some word $\zeta \in (A \setminus V)^\omega$, then all such ζ satisfy f_1, and the clause $(\mathbf{G}\neg\hat{V}) \wedge \mathbf{X}\beta(f_1)$ can be replaced by $\mathbf{G}\neg\hat{V}$. Otherwise, that clause can be removed altogether. One can determine whether a formula is satisfied by such a word by replacing every occurrence of every action with false.

3.3 Generation of Interruptible LTL Formulas

The following can be used to show that many formulas are interruptible. It establishes a kind of parity pattern involving a class of *positive* formulas (Pos) and a class of *negative* formulas (Neg). It is proved in [28].

Proposition 5. *There exist* $\mathsf{Pos}, \mathsf{Neg} \subseteq \mathsf{Form}$ *such that (i) for all* $f, f' \in \mathsf{Form}$,

$$(f \in \mathsf{Pos} \wedge f' \equiv_{\mathsf{A}} f) \Rightarrow f' \in \mathsf{Pos}$$
$$(f \in \mathsf{Neg} \wedge f' \equiv_{\mathsf{A}} f) \Rightarrow f' \in \mathsf{Neg},$$

and (ii) for all $a \in \mathsf{Act}$, $f_1, f_2 \in \mathsf{Intrpt}$, $g_1, g_2 \in \mathsf{Pos}$, *and* $h_1, h_2 \in \mathsf{Neg}$,

$$\textit{false},\ a,\ \neg h_1,\ g_1 \wedge g_2,\ g_1 \vee g_2,\ a \wedge f_1,\ a \wedge \mathbf{X}f_1 \ \in\ \mathsf{Pos}$$
$$\textit{true},\ \neg a,\ \neg g_1,\ h_1 \wedge h_2,\ h_1 \vee h_2,\ \neg a \vee f_1,\ \neg a \vee \mathbf{X}f_1 \ \in\ \mathsf{Neg}$$
$$\textit{true},\ \textit{false},\ f_1 \wedge f_2,\ f_1 \vee f_2,\ \neg f_1,\ \mathbf{F}g_1,\ \mathbf{G}h_1,\ f_1\mathbf{U}f_2,\ h_1\mathbf{U}g_1,\ h_1\mathbf{U}f_1 \ \in\ \mathsf{Intrpt}.$$

Consider the examples from Sect. 3.1. The formula a is positive, so $\mathbf{F}a$ is interruptible. Since $\neg a$ is negative, $\mathbf{G}\neg a$ is interruptible. Since $\mathbf{F}a$ is interruptible, $a \wedge \mathbf{XF}a$ is positive, hence $\mathbf{F}(a \wedge \mathbf{XF}a)$ is interruptible.

Formula $\mathbf{G}(a \rightarrow \mathbf{F}b)$ is seen to be interruptible as follows. Since $b \in \mathsf{Pos}$, $\mathbf{F}b \in \mathsf{Intrpt}$, whence $\neg a \vee \mathbf{F}b \in \mathsf{Neg}$. Since this last formula is action-equivalent to $a \rightarrow \mathbf{F}b$, we have $a \rightarrow \mathbf{F}b \in \mathsf{Neg}$. Therefore $\mathbf{G}(a \rightarrow \mathbf{F}b) \in \mathsf{Intrpt}$.

Similarly, $(\neg b)\mathbf{U}c \in \mathsf{Intrpt}$, so $a \rightarrow \mathbf{X}((\neg b)\mathbf{U}c) \in \mathsf{Neg}$. This negative formula is action-equivalent to $a \rightarrow ((\neg b)\mathbf{U}c)$, whence $\mathbf{G}(a \rightarrow ((\neg b)\mathbf{U}c)) \in \mathsf{Intrpt}$.

Note that Intrpt and the set of stutter-invariant formulas are not comparable. For example, $f = \mathbf{F}(a \wedge \mathbf{XF}a)$ is interruptible, but not stutter-invariant. In fact f is not action-equivalent to any stutter-invariant formula g, since if there were such a g, the sequence aab^ω would satisfy g, but the stutter-equivalent sequence ab^ω cannot satisfy g. Conversely, the formulas a and $\mathbf{G}a$ are both stutter-invariant, but neither is interruptible. The formula $\mathbf{F}a$ is both stutter-invariant and interruptible. Finally, the formula $\mathbf{X}a$ is neither stutter-invariant nor interruptible.

3.4 Decidability of Interruptibility of Büchi Automata

Definition 11. Let B be a BA with alphabet A, $V \subseteq A$ (the *visible* actions), and $I = A \setminus V$ (the *invisible actions*). We say B is in *V-interrupt normal form* if the following hold for any $x \in I$, $a \in A$, and states s_1, s_2, and s_3:

1. If $s_1 \xrightarrow{a} s_2$ then B has a state s_1' such that $s_1 \xrightarrow{x} s_1' \xrightarrow{a} s_2$.
2. If $s_1 \xrightarrow{x} s_2 \xrightarrow{a} s_3$ then $s_1 \xrightarrow{a} s_3$ and if s_2 is accepting then s_1 or s_3 is accepting.
3. If $s_1 \xrightarrow{x} s_2$ then $s_1 \xrightarrow{y} s_2$ for all $y \in I$.

Proposition 6. *Suppose B is in V-interrupt normal form. Then $\mathcal{L}(B)$ is V-interruptible.*

Proof. Suppose $\zeta, \eta \in A^\omega$, $\zeta \in \mathcal{L}(B)$, and $\zeta|_V = \eta|_V$. We wish to show $\eta \in \mathcal{L}(B)$. Let π be an accepting path for ζ.

Assume $\zeta|_V$ is infinite. By Definition 11(2), we can remove all invisible transitions from the accepting path π, and the result is an accepting path that spells $\zeta|_V$. By Definition 11(1), we can insert any arbitrary finite sequence of invisible transition between two consecutive visible transitions; we can therefore construct an accepting path for η.

If $\zeta|_V$ is finite, proceed as above to form an accepting path which spells a finite prefix of η followed by an infinite word of invisible actions. By Definition 11(3), that infinite suffix can be transformed to spell any infinite word of invisibles, and in that way one obtains an accepting path for η. □

Given any BA $B = (S, A, T, S^0, F)$ and a visible set $V \subseteq A$, define a BA $\mathsf{norm}(B, V)$ as follows: if $V = A$, $\mathsf{norm}(B, V) = B$, otherwise $\mathsf{norm}(B, V)$ is $\hat{B} = (\hat{S}, A, \hat{T}, \hat{S}^0, \hat{F})$, where

$$
\begin{aligned}
D &= \{s \in S \mid \text{there is an accepting path from } s \text{ with all labels in } I\} \\
\hat{S} &= \{\hat{u} \mid u \in S\} \cup \{u^\sharp \mid u \in F \setminus D\} \cup \{\mathsf{DIV}\} \\
\hat{S}^0 &= \{\hat{u} \mid u \in S^0\} \\
\hat{F} &= \{\hat{u} \mid u \in F\} \cup \{\mathsf{DIV}\} \\
\hat{T} = &\begin{array}{lll}
\{(\hat{u}, a, \hat{v}) & \mid a \in V \wedge u, v \in S \wedge (u, a, v) \in T & \} \cup \\
\{(\hat{u}, x, \hat{u}) & \mid x \in I \wedge u \in D \cup (S \setminus F) & \} \cup \\
\{(\mathsf{DIV}, x, \mathsf{DIV}) & \mid x \in I & \} \cup \\
\{(\hat{u}, x, \mathsf{DIV}) & \mid x \in I \wedge u \in D \setminus F & \} \cup \\
\{(\hat{u}, x, u^\sharp), (u^\sharp, x, u^\sharp) & \mid x \in I \wedge u \in F \setminus D & \} \cup \\
\{(u^\sharp, a, \hat{v}) & \mid a \in V \wedge u \in F \setminus D \wedge v \in S \wedge (u, a, v) \in T & \}
\end{array}
\end{aligned}
$$

The set $\hat{S}$ consists of the *original states* $\hat{u}$, the *sharp states* $u^\sharp$, and one additional state DIV. The mapping from S to $\hat{S}$ defined by $u \mapsto \hat{u}$ is injective and preserves acceptability and visible transitions, i.e., for any $u, v \in S$ and $a \in V$, $u \xrightarrow{a} v \;\Leftrightarrow\; \hat{u} \xrightarrow{a} \hat{v}$. It follows that paths in B in which all labels are visible correspond one-to-one with paths through original states in $\hat{B}$ in which all labels are visible. Note that every invisible transition in $\hat{B}$ is a self-loop or ends in a sharp state or DIV. Moreover, all transitions in $\hat{B}$ ending in a sharp state or DIV are invisible.

Proposition 7. *For any BA B with alphabet A, and any visible set $V \subseteq A$, $\mathsf{norm}(B, V)$ is in V-interrupt normal form.*

Proof. To see Definition 11(1), suppose $s_1 \xrightarrow{a} s_2$. If $s_1 \xrightarrow{x} s_1$, take $s_1' = s_1$. Otherwise, $s_1 = \hat{u}$ for some $u \in F \setminus D$, and we can take $s_1' = u^\sharp$.

For Definition 11(2), suppose $s_1 \xrightarrow{x} s_2 \xrightarrow{a} s_3$. We need to show $s_1 \xrightarrow{a} s_3$ and if s_2 is accepting then s_1 or s_3 is accepting. If $s_1 = s_2$, the result is clear, so assume $s_1 \neq s_2$. There are then two cases: $s_2 = \mathsf{DIV}$ or $s_2 = u^\sharp$ for some $u \in F \setminus D$.

If $s_2 = \mathsf{DIV}$, then $a \in I$ and $s_3 = \mathsf{DIV}$, and we have $s_1 \xrightarrow{a} \mathsf{DIV}$. As DIV is accepting, the desired conclusion holds.

If $s_2 = u^\sharp$, then $s_1 = \hat{u}$, which is accepting. There are again two cases: either $s_3 = u^\sharp$ or $s_3 = \hat{v}$ for some $v \in S$. If $s_3 = u^\sharp$ then $a \in I$ and $\hat{u} \xrightarrow{a} u^\sharp$, as required. If $s_3 = \hat{v}$, then $a \in V$ and therefore $u \xrightarrow{a} v$, hence $\hat{u} \xrightarrow{a} \hat{v}$, as required.

Definition 11(3) is clear from the definition of $\hat{T}$. □

Theorem 2. *$\mathcal{L}(B)$ is V-interruptible iff $\mathcal{L}(\mathsf{norm}(B, V)) = \mathcal{L}(B)$. In particular interruptibility for Büchi Automata is decidable.*

Proof. Let $P_1 = \mathcal{L}(B)$ and $P_2 = \mathcal{L}(\mathsf{norm}(B, V))$. By Proposition 7, $\mathsf{norm}(B, V)$ is in V-interrupt normal form, so by Proposition 6, P_2 is V-interruptible. Hence one direction is clear: if $P_1 = P_2$, then P_1 is V-interruptible.

So suppose P_1 is V-interruptible. We wish to show $P_1 = P_2$. By Lemma 2, it suffices to show the two languages contain the same V-interrupt-free words.

Suppose ζ is a V-interrupt-free word in P_1. If $\zeta \in V^\omega$ then an accepting path θ in B maps to the accepting path $\hat{\theta}$ in $\hat{B}$, and $\zeta \in P_2$. So assume $\zeta \in V^* I^\omega$. Then an accepting path in B has a prefix θ of visible transitions ending in a state $u \in D$. That prefix corresponds to a path $\hat{\theta}$ in $\hat{B}$ ending in $\hat{u}$. As $u \in D$, $\hat{u} \xrightarrow{x} \hat{u}$ for all $x \in I$. If u is accepting, we get an accepting path for ζ that follows $\hat{\theta}$ and then loops at $\hat{u}$. If u is not accepting then $u \in D \setminus F$, and $\hat{u} \xrightarrow{x} \mathsf{DIV}$ for all $x \in I$. Since DIV is accepting and $\mathsf{DIV} \xrightarrow{x} \mathsf{DIV}$ for all $x \in I$, we again get an accepting path for ζ in $\hat{B}$.

Suppose now that ζ is a V-interrupt-free word in P_2. Assume $\zeta \in V^\omega$. An accepting path for ζ cannot pass through a sharp state or DIV, because only invisible transitions end in those states. So the path passes through only original states, and therefore corresponds to an accepting path in B.

Suppose $\zeta \in V^* I^\omega$. An accepting path for ζ in $\hat{B}$ consists of a prefix $\hat{\theta}$ of visible transitions followed by an infinite accepting path ξ of invisible transitions. As above, $\hat{\theta}$ corresponds to a path θ in B ending in a state u.

We claim that ξ cannot pass through a sharp state. This is because all invisible transitions departing from a sharp state are self loops. But sharp states are not accepting, while ξ is an accepting path of invisible transitions. It follows that each transition in ξ is a self-loop or terminates in DIV.

We now claim $u \in D$. For suppose the first transition in ξ is a self-loop on $\hat{u}$. According to the definition of $\hat{T}$, this implies $u \in D \cup (S \setminus F)$. Hence, if $u \notin D$ then u is not accepting, and all invisible transitions departing from $\hat{u}$ are self-loops, contradicting the fact that ξ is an accepting path. If, on the other hand, the first transition in ξ is $\hat{u} \xrightarrow{x} \mathsf{DIV}$, for some $x \in I$, then the definition of $\hat{T}$ implies $u \in D$, establishing the claim.

So $u \in D$, i.e., there is an accepting path ρ in B starting from u and consisting of all invisible transitions. The accepting path obtained by concatenating θ and ρ spells a word which, projected onto V, equals $\zeta|_V$. Since P_1 is V-interruptible, $\zeta \in P_1$. This completes the proof that $P_1 = P_2$.

The theorem reduces the problem of determining V-interruptibility to a problem of determining equivalence of two Büchi Automata, which can be done using language intersection, complement, and emptiness algorithms for BAs [37]. □

4 On-the-Fly Partial Order Reduction

4.1 General Theory and Soundness Theorem

Let $M = (Q, A, T, q^0)$ be an LTS, $V \subseteq A$, and $B = (S, A, \delta, S^0, F)$ a V-interruptible BA. The goal of on-the-fly POR is to explore a sub-automaton R' of $R = M \parallel B$ with the property that $\mathcal{L}(R) = \emptyset \Leftrightarrow \mathcal{L}(R') = \emptyset$.

A function $\mathsf{amp}\colon Q \times S \to 2^A$ is an *ample selector* if $\mathsf{amp}(q, s) \subseteq \mathsf{enabled}(M, q)$ for all $q \in Q, s \in S$. Each $\mathsf{amp}(q, s)$ is an *ample set*. An ample selector determines a BA $R' = \mathsf{reduced}(R, \mathsf{amp})$ which has the same states, accepting states, and initial state as R, but only a subset of the transitions:

$$R' = (Q \times S, A, \delta', \{q^0\} \times S^0, Q \times F)$$
$$\delta' = \{((q, s), a, (q', s')) \mid a \in \mathsf{amp}(q, s) \wedge (q, a, q') \in T \wedge (s, a, s') \in \delta\}.$$

We now define some constraints on an ample selector that will be used to guarantee the reduced product space has nonempty language if the full space does. First we need the usual notion of independence:

Definition 12. Let M be an LTS with alphabet A, and $a, b \in A$. We say a and b are *independent* if both of the following hold for all states q and q' of M:

1. $(q \xrightarrow{a} q' \wedge b \in \mathsf{enabled}(M, q)) \Rightarrow b \in \mathsf{enabled}(M, q')$
2. $q \xrightarrow{ab} q' \Leftrightarrow q \xrightarrow{ba} q'$.

We say a and b are *dependent* if they are not independent. □

Note that, in contrast with [1], we do not assume actions are deterministic. We can now define the four constraints:

C0 For all $q \in Q$, $s \in S$: $\mathsf{enabled}(M, q) \neq \emptyset \Rightarrow \mathsf{amp}(q, s) \neq \emptyset$.
C1 For all $q \in Q$, $s \in S$: on any trace in M starting from q, no action outside of $\mathsf{amp}(q, s)$ but dependent on an action in $\mathsf{amp}(q, s)$ can occur without an action in $\mathsf{amp}(q, s)$ occurring first.
C2 For all $q \in Q$, $s \in S$: if $\mathsf{amp}(q, s) \neq \mathsf{enabled}(M, q)$, then $\mathsf{amp}(q, s) \cap V = \emptyset$.
C3 For all $a \in A$: on any cycle in R' for which a is enabled in R at each state, there is some state (q, s) on the cycle for which $a \in \mathsf{amp}(q, s)$.

Theorem 3. *Let M be an LTS with alphabet A, $V \subseteq A$, B a BA with alphabet A in V-interrupt normal form, $R = M \parallel B$, and* amp *an ample selector satisfying* **C0**–**C3**. *Then $\mathcal{L}(\mathsf{reduced}(R, \mathsf{amp})) = \emptyset \Leftrightarrow \mathcal{L}(R) = \emptyset$.*

The requirement that B be in interrupt normal form is necessary. A counterexample when that condition is not met is given in Fig. 1. Note a and b are independent, and a is invisible. The ample set for product states 0 and 1 is $\{a\}$; the ample set for product state 2 is $\{a, b\}$. Hence **C3** holds because a state on the sole cycle is fully enabled. After normalizing B (and removing unreachable states), this problem goes away: in any reduced space, the ample sets must retain

the a-transitions, and state $0^\sharp$ must be fully enabled since it has an a-self-loop, so the accepting cycle involving the two states will remain.

The remainder of this section is devoted to the proof of Theorem 3. The proof is similar to that of the analogous theorem in the state-based case [27], but some changes are necessary and we include the proof for completeness.

Let θ be an accepting path in R. An infinite sequence of accepting paths $\pi_0, \pi_1, \ldots$ will be constructed, where $\pi_0 = \theta$. For each $i \geq 0$, π_i will be decomposed as $\eta_i \circ \theta_i$, where η_i is a finite path of length i in R', θ_i is an infinite path, and η_i is a prefix of η_{i+1}. For $i = 0$, η_0 is empty and $\theta_0 = \theta$.

Assume $i \geq 0$ and we have defined η_j and θ_j for $j \leq i$. Write

$$\theta_i \;=\; \langle q_0, s_0\rangle \xrightarrow{a_1} \langle q_1, s_1\rangle \xrightarrow{a_2} \cdots \tag{1}$$

Then η_{i+1} and θ_{i+1} are defined as follows. Let $E = \mathsf{amp}(q_0, s_0)$. There are two cases:

Case 1: $a_1 \in E$. Let η_{i+1} be the path obtained by appending the first transition of θ_i to η_i, and θ_{i+1} the path obtained by removing the first transition from θ_i.

Case 2: $a_1 \notin E$. Then there are two sub-cases:

Case 2a: Some operation in E occurs in θ_i. Let n be the index of the first such occurrence. By **C1**, a_j and a_n are independent for $1 \leq j < n$. By repeated application of the independence property, there is a path in M of the form

$$q_0 \xrightarrow{a_n} q'_1 \xrightarrow{a_1} q'_2 \xrightarrow{a_2} \cdots \xrightarrow{a_{n-2}} q'_{n-1} \xrightarrow{a_{n-1}} q_n \xrightarrow{a_{n+1}} q_{n+1} \xrightarrow{a_{n+2}} \cdots .$$

By **C2**, a_n is invisible. By Definition 11, B has an accepting path of the form

$$s_0 \xrightarrow{a_n} s'_0 \xrightarrow{a_1} s_1 \xrightarrow{a_2} \cdots \xrightarrow{a_{n-2}} s_{n-2} \xrightarrow{a_{n-1}} s_{n-1} \xrightarrow{a_{n+1}} s_{n+1} \xrightarrow{a_{n+2}} \cdots .$$

Composing these two paths yields a path in R. Removing the first transition (labeled a_n) yields θ_{i+1}. Appending that transition to η_i yields η_{i+1}.

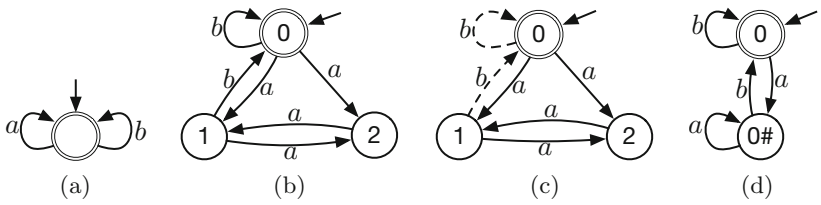

Fig. 1. Counterexample to Theorem 3 if B is not in interrupt normal form: (a) the LTS M, (b) the BA B representing $\mathbf{GF}b$, (c) the product space—dashed edges are in the full, but not reduced, space, and (d) the result of normalizing B and removing unreachable states, which also depicts the resulting full product space.

Case 2b: No operation in E occurs in θ_i. By **C0**, E is nonempty. Let $b \in E$. By **C2**, every action in θ_i is independent of b. As in the case above, we obtain a path in R

$$\langle q_0, s_0\rangle \xrightarrow{b} \langle q_1', s_0'\rangle \xrightarrow{a_1} \langle q_2', s_1\rangle \xrightarrow{a_2} \langle q_3', s_2\rangle \xrightarrow{a_3} \cdots .$$

and define θ_{i+1} and η_{i+1} as above.

Let η be the limit of the η_i, i.e., $\eta(i) = \eta_{i+1}(i)$. It is clear that η is an infinite path in R', but we must show it passes through an accepting state infinitely often. To see this, define integers d_i for $i \geq 0$ as follows. Let $\xi_i = s_0 s_1 \cdots$ be the sequence of BA states traced by θ_i. Let d_i be the minimum $j \geq 0$ such that s_j is accepting. Note that $d_i = 0$ iff $\mathsf{last}(\eta_i)$ is accepting.

Suppose $i \geq 0$ and $d_i > 0$. If Case 1 holds, then $d_{i+1} = d_i - 1$, since $\xi_{i+1} = \xi_i^1$. It is not hard to see that if Case 2 holds, $d_{i+1} \leq d_i$. Note that in Case 2a, if $d_i = n$, the accepting state s_n is removed, but Definition 11(2) guarantees that at least one of s_{n-1} and s_{n+1} is accepting. In the worst case (s_{n-1} is not accepting), we still have $d_{i+1} = n$.

We claim there are an infinite number of $i \geq 0$ such that Case 1 holds. Otherwise, there is some $i > 0$ such that Case 2 holds for all $j \geq i$. Let a be the first action in θ_i. Then for all $j \geq i$, a is the first action of θ_j and a is not in the ample set of $\mathsf{last}(\eta_j)$. Since the number of states of R is finite, there is some $k > i$ such that $\mathsf{last}(\eta_k) = \mathsf{last}(\eta_i)$. Hence there is a cycle in R' for which a is always enabled but never in the ample set, contradicting **C3**.

If η does not pass through an accepting state infinitely often, there is some $i \geq 0$ such that for all $j \geq i$, $\mathsf{first}(\theta_j)$ is not accepting. But then $(d_j)_{j \geq i}$ is a nondecreasing sequence of positive integers which strictly decreases infinitely often, a contradiction.

4.2 Ample Sets for a Parallel Composition of LTSs

We now describe the specific method used by McRERS to select ample sets. Since this method is similar to existing approaches, such as [32, Algorithm 4.3], we just outline the main ideas.

Let $n \geq 1$, $P = \{1, \ldots, n\}$, and let $M_1, \ldots, M_n$ be LTSs over Act. Write $M_i = (Q_i, A_i, \rightarrow_i, q_i^0)$ and

$$M = M_1 \parallel \cdots \parallel M_n = (Q, A, \rightarrow, q^0).$$

For $a \in A$, let $\mathsf{procs}(a) = \{i \in P \mid a \in A_i\}$. It can be shown that if a and b are dependent actions, then $\mathsf{procs}(a) \cap \mathsf{procs}(b) \neq \emptyset$.

Let $q = (q_1, \ldots, q_n) \in Q$ and $E_i = \mathsf{enabled}(M_i, q_i)$ for $i \in P$. Let

$$R_q = \{(i, j) \in P \times P \mid E_i \cap A_j \neq \emptyset\}.$$

Suppose $C \subseteq P$ is closed under R_q, i.e., for all $i \in C$ and $j \in P$, $(i, j) \in R_q \Rightarrow j \in C$. This implies that if $a \in E_i$ for some $i \in C$ then $\mathsf{procs}(a) \subseteq C$. Define

$$\mathsf{enabled}(C, q) = \mathsf{enabled}(M, q) \cap \bigcup_{i \in C} A_i.$$

Let $E = \mathsf{enabled}(C, q)$. Note $E \subseteq \bigcup_{i \in C} E_i$. Hence for any $a \in E$, $\mathsf{procs}(a) \subseteq C$.

Lemma 3. *On any trace in M starting from q, no action outside of E but dependent on an action in E can occur without an action in E occurring first.*

Proof. Let ζ be a trace in M starting from q, such that no element of E occurs in ζ. We claim no action involving C (i.e., an action a for which $\mathsf{procs}(a) \cap C \neq \emptyset$) can occur in ζ. Otherwise, let x be the first such action. Then $x \in E_i$, for some $i \in C$, so $\mathsf{procs}(x) \subseteq C$. As $x \notin E$, $x \notin \mathsf{enabled}(M, q)$. So some earlier action y in ζ caused x to become enabled, and therefore $\mathsf{procs}(x) \cap \mathsf{procs}(y) \neq \emptyset$, hence $\mathsf{procs}(y) \cap C \neq \emptyset$, contradicting the assumption that x was the first action involving C in ζ.

Now any action b dependent on an action $a \in E$ must satisfy $\mathsf{procs}(a) \cap \mathsf{procs}(b)$ is nonempty. Since $\mathsf{procs}(a) \subseteq C$, $\mathsf{procs}(b) \cap C$ is nonempty. Hence no action dependent on an action in E can occur in ζ. □

We now describe how to find an ample set in the context of NDFS. Let (q, s) be a new product state that has just been pushed onto the outer DFS stack. The relation R_q defined above gives P the structure of a directed graph. Suppose that graph has a strongly connected component C_0 such that all of the following hold for $E = \mathsf{enabled}(C_0, q)$:

1. $E \neq \emptyset$,
2. $E \cap V = \emptyset$,
3. $\mathsf{enabled}(C', q) = \emptyset$ for all SCCs C' reachable from C_0 other than C_0, and
4. E does not contain a "back edge", i.e., if $(q, s) \xrightarrow{a} \sigma$ for some $a \in E$ and $\sigma \in Q \times S$, then σ is not on the outer DFS stack.

Then set $\mathsf{amp}(q, s) = E$. If no such SCC exists, set $\mathsf{amp}(q, s) = \mathsf{enabled}(M, q)$. It follows that **C0**–**C4** hold. Note that the union C of all SCCs reachable from C_0 is closed under R_q, and $\mathsf{enabled}(C, q) = E$, so Lemma 3 guarantees **C1**. For **C3**, we actually have the stronger condition that in any cycle in the reduced space, at least one state is fully enabled. In our implementation, the SCCs are computed using Tarjan's algorithm. Among all SCCs C_0 satisfying the conditions above, we choose one for which $|\mathsf{enabled}(C_0, q)|$ is minimal.

One known issue when combining NDFS with on-the-fly POR is that the inner DFS must explore the same subspace as the outer DFS, i.e., amp must be a deterministic function of its input (q, s) [18]. To accomplish this, McRERS stores one additional integer j in the state: j is the root node of the SCC C_0, or -1 if the state is fully enabled. The outer search saves j in the state, and the inner search uses j to reconstruct the SCC C_0 and the ample set E.

5 Related Work

There has been significant earlier research on the use of partial order reduction to model check LTSs (or the closely related concept of process algebras); see, e.g., [14,16,30–33,35]. To understand how this previous work relates to this paper,

we must explain a subtle, but important, distinction concerning how a property is specified. In much of this literature, a property of an LTS with alphabet A is essentially a pair $\pi = (V, T)$, where $V \subseteq A$ is a set of visible actions and T is a set of (finite and infinite) words over V. A property in this sense specifies acceptable behaviors *after invisible actions have been removed*. (See, e.g., Def. 2.4 and preceding comments in [32].) We can translate π to a property P in our sense by taking its inverse image under the projection map:

$$P = \{\zeta \in A^\omega \mid \zeta|_V \in T\}.$$

Note that P *is* V*-interruptible by definition*. Hence the need to distinguish interruptible properties does not arise in this context.

Much of the earlier work on POR for LTSs deals with the "offline" case, i.e., the construction of a subspace of M that preserves certain classes of properties. In contrast, Theorem 3 deals with an on-the-fly algorithm, i.e., the construction of a subspace of $M \parallel B$. The on-the-fly approach is an essential optimization in model checking, but recent work in the state-based formalism has shown that offline POR schemes do not always generalize easily to on-the-fly algorithms [27].

One work that does describe an on-the-fly model checking algorithm for LTSs is [32] (see also [17], which deals with the same ideas in a state formalism). The property is specified by a *tester process* B. Consistent with the notion of *property* described above, the alphabet of B does not include the invisible actions. Hence, in the parallel composition $M \parallel B$, the tester does not move when M executes an invisible action. In order to specify both finite and infinite words of visible actions, the tester has two kinds of accepting states: "livelock monitor states" and "infinite trace monitor states." (Two additional classes of states for detecting other kinds of violations are not relevant to the discussion here.) A version of the stubborn set theory is used to define the reduced space, and a special condition is used to solve the "ignoring problem" (instead of our **C3**). It would be interesting to compare this algorithm with the one described here.

There are many algorithms for reducing or even minimizing the size of an LTS while preserving various properties, e.g., *bisimulation equivalence* [8] or *divergence preserving bisimilarity* [6]. These algorithms could be applied to the individual components of a parallel composition (taking all visible and communication actions to be "visible"), as a preprocessing step before beginning the model checking search. An exploration of these algorithms, and how they impact POR, is beyond the scope of this paper, but we hope to explore that avenue in future work.

The RERS Challenge [9,19–21] is an annual event involving a number of different categories of large model checking problems. The "parallel LTL category," offered from 2016 on, is directly relevant to this paper. Each problem in that category consists of a Graphviz "dot" file specifying an LTS as a parallel composition, and a text file containing 20 LTL formulas. The goal is to identify the formulas satisfied by the LTS. The solutions are initially known only to the organizers, and are published after the event. The RERS semantics for LTSs, LTL, and satisfiability are exactly the same as in this paper.

The methods for generating the LTS and the properties are complicated, and have varied over the years, but are designed to satisfy certain hardness guarantees. The approach described in [29] is "... based on the weak refinement ... of convergent systems which preserves an interesting class of temporal properties." It can be seen that the properties preserved by weak refinement are exactly the interruptible properties. While [29] does not describe a method for determining whether a property is interruptible, the authors have informed us that they developed a sufficient condition for an LTL formula to be interruptible, and used this in combination with a random method to generate the formulas for 2016 and 2019. Our analysis (Sect. 6) confirms that all formulas from 2016 and 2019 are interruptible, while 2017 and 2018 contain some non-interruptible formulas.

There is a well-known way to translate a system and property expressed in an action-based formalism to a state-based formalism. The idea is to add a shared variable *last* which records the last action executed. An LTL formula over actions can be transformed to one over states by replacing each action a with the predicate $last = a$. This is the approach taken in the Promela representations of the parallel problems provided with the RERS challenges.

This translation is semantics-preserving but performance-destroying. Every transition writes to the shared variable *last*, so any state-based POR scheme will assume that no two transitions commute. Furthermore, since the property references *last*, all transitions are visible. This effectively disables POR, even when the property is stutter-invariant, as can be seen in the poor performance of Spin on the RERS Promela models (Sect. 6). It is possible that there are more effective Spin translations; [34, §2.2], for example, suggests not updating *last* on invisible actions, and adding a global boolean variable that is flipped on every visible action (in addition to updating *last*). We note that this would also require modifying the LTL formula, or specifying the property in some other way. In any case, it suggests another interesting avenue for future work.

6 Experimental Results and Conclusions

We implemented a model checker named McRERS based on the algorithms described in this paper. McRERS is a library and set of command line tools. It is written in sequential C and uses the Spot library [4] for several tasks: (1) determining equivalence of LTL formulas, (2) determining language equivalence of BAs, and (3) converting an LTL formula to a BA. The source code for McRERS as well as all artifacts related to the experiments discussed in this section, are available at https://vsl.cis.udel.edu/cav2020. The experiments were run on an 8-core 3.7GHz Intel Xeon W-2145 Linux machine with 256 GB RAM, though McRERS is a sequential program and most experiments required much less memory.

As described in Sect. 5, each edition of RERS includes a number of problems, each of which comes with 20 LTL formulas. The numbers of problems for years 2016–2019 are, in order, 20, 15, 3, and 9, for a total of 47 problems, or $47 * 20 = 940$ distinct model checking tasks. (Some formulas become identical

after renaming propositions.) We used the McRERS *property analyzer* to analyze these formulas to determine which are interruptible; the algorithm used is based on Theorem 1. The results show that all formulas from 2016 and 2019 are interruptible, which agrees with the expectations of the RERS organizers. In 2017, 22 of the 300 formulas are not interruptible; these include

- $\mathbf{GF}\neg\texttt{a111\_SIGTRAP}$,
- $\mathbf{G}[\texttt{a71\_SIGVTALRM} \rightarrow \mathbf{X}\neg\texttt{a71\_SIGVTALRM}]$, and
- $\mathbf{G}[(\texttt{a59\_SIGUSR1} \wedge \mathbf{X}[(\neg\texttt{a112\_SIGHUP})\mathbf{U}\texttt{a59\_SIGUSR1}]) \rightarrow \mathbf{FG}\texttt{a104\_SIGPIPE}]$.

In 2018, 3 of the 60 formulas are not interruptible. In summary, only 25 of the 940 tasks involve non-interruptible formulas. The total runtime for the analysis of all 940 formulas was 6 s.

We next used the McRERS *automaton analyzer* to create BAs from each of the interruptible formulas, and then to determine which of these Spot-generated BAs was not in interrupt normal form. This uses a straightforward algorithm that iterates over all states and checks the conditions of Definition 11. For each BA not in normal form, the analyzer transforms it to normal form using function norm of Sect. 3.4. Interestingly, all of the Spot-generated BAs in 2016 and 2019 were already in normal form. Four of the BAs from interruptible formulas in 2017 were not in normal form; all of these formulas had the form $\mathbf{F}[a \vee ((\neg b)\mathbf{W}c)]$. In 2018, 6 interruptible formulas have non-normal BAs; these formulas have several different non-isomorphic forms, some of which are quite complex. The details can be seen on the online archive. The total runtime for this analysis (including writing all BAs to a file) was 11 s.

The McRERS model checker parses RERS "dot" and property files to construct an internal representation of a parallel composition $M = M_1 \parallel \cdots \parallel M_n$ of LTSs and a list of LTL formulas. Each formula f is converted to a BA B; if f is interruptible and B is not already in normal form, B is transformed to normal form. The NDFS algorithm is used to determine language emptiness, and if f is interruptible, the POR scheme described in Sect. 4 is also used. States are saved in a hash table.

One other simple optimization is used regardless of whether f is interruptible. Let αM denote the set of actions labeling at least one transition in M, and define αB similarly. If $\alpha M \neq \alpha B$, then all transitions labeled by an action in $(\alpha M \setminus \alpha B) \cup (\alpha B \setminus \alpha M)$ are removed from the M_i and B; all unreachable states and transitions in the M_i and B are also removed. This is repeated until $\alpha M = \alpha B$.

We applied the model checker to all problems in the 2019 benchmarks. Interestingly, all 180 tasks completed, with the correct results, using at most 8 GB RAM; the times are given in Fig. 2.

We also ran these problems with POR turned off, to measure the impact of that optimization. As is often the case with POR schemes, the difference is dramatic. The non-POR tests ran out of memory on our 256 GB machine after problem 106. We show the resources consumed for a representative task in Fig. 3; this property holds, so a complete search is required. In terms of number of states or time, the performance differs by about 5 orders of magnitude.

Problem	101	102	103	104	105	106	107	108	109
Components	8	10	12	15	20	25	50	60	70
Time (s)	1	1	1	1	1	1	14	54	432

Fig. 2. Time to solve RERS 2019 parallel LTL problems using McRERS. Each problem comprises 20 LTL formulas. Memory limited to 8 GB. Rows: problem number, number of components in the LTS, and total McRERS wall time rounded up to nearest second.

POR?	States saved	Transitions	Memory (MB)	Time (s)
YES	1.55×10^4	1.55×10^4	1.26×10^2	< 0.1
NO	1.89×10^9	1.35×10^{10}	2.61×10^5	7865.0

Fig. 3. Performance impact of POR on solving RERS 2019 problem 106, formula 1, $(\texttt{a6} \rightarrow \mathbf{F}\texttt{a7})\mathbf{W}(\texttt{a7} \vee \texttt{a88})$.

Tool	States	Transitions	Memory(MB)	Time(s)
Spin	8.16×10^7	2.01×10^8	1.09×10^4	292.0
McRERS	1.80×10^2	1.93×10^2	5.06×10^1	< 0.1

Fig. 4. Performance of Spin v6.5.1 and McRERS on RERS 2019 problem 101, property 1. Both tools used POR. Spin used `-DCOLLAPSE` for state compression and `-m100000000` for search depth bound.

As explained in Sect. 5, the RERS Spin models can not be expected to perform well. We ran the latest version of Spin on these using `-DCOLLAPSE` compression. We show the result for just the first task in Fig. 4. There is at least a 4 order of magnitude performance difference (measured in states or time) between the tools. An examination of Spin's output in verbose mode reveals the problem to be as described in Sect. 5: the full set of enabled transitions is explored at each transition due to the update of the shared variable.

The 2016 RERS problems are more challenging for McRERS. The problems are numbered from 101 to 120. To scale beyond problem 111, with a memory bound of 256 GB, additional reduction techniques, such as the component minimization methods discussed in Sect. 5, must be used. We plan to carry out a thorough study of those methods and how they interact with POR.

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Global Guidance for Local Generalization in Model Checking

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Abstract. SMT-based model checkers, especially IC3-style ones, are currently the most effective techniques for verification of infinite state systems. They infer *global* inductive invariants via *local* reasoning about a single step of the transition relation of a system, while employing SMT-based procedures, such as interpolation, to mitigate the limitations of local reasoning and allow for better generalization. Unfortunately, these mitigations intertwine model checking with heuristics of the underlying SMT-solver, negatively affecting stability of model checking.

In this paper, we propose to tackle the limitations of locality in a systematic manner. We introduce explicit *global guidance* into the local reasoning performed by IC3-style algorithms. To this end, we extend the SMT-IC3 paradigm with three novel rules, designed to mitigate fundamental sources of failure that stem from locality. We instantiate these rules for the theory of Linear Integer Arithmetic and implement them on top of Spacer solver in Z3. Our empirical results show that GSpacer, Spacer extended with global guidance, is significantly more effective than both Spacer and sole global reasoning, and, furthermore, is insensitive to interpolation.

1 Introduction

SMT-based Model Checking algorithms that combine SMT-based search for bounded counterexamples with interpolation-based search for inductive invariants are currently the most effective techniques for verification of infinite state systems. They are widely applicable, including for verification of synchronous systems, protocols, parameterized systems, and software.

The Achilles heel of these approaches is the mismatch between the *local* reasoning used to establish absence of bounded counterexamples and a *global* reason for absence of unbounded counterexamples (i.e., existence of an inductive invariant). This is particularly apparent in IC3-style algorithms [7], such as Spacer [18]. IC3-style algorithms establish bounded safety by repeatedly computing predecessors of error (or bad) states, blocking them by local reasoning

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about a single step of the transition relation of the system, and, later, using the resulting *lemmas* to construct a candidate inductive invariant for the global safety proof. The whole process is driven by the choice of local lemmas. Good lemmas lead to quick convergence, bad lemmas make even simple-looking problems difficult to solve.

The effect of local reasoning is somewhat mitigated by the use of interpolation in lemma construction. In addition to the usual inductive generalization by dropping literals from a blocked bad state, interpolation is used to further generalize the blocked state using theory-aware reasoning. For example, when blocking a bad state $x = 1 \wedge y = 1$, inductive generalization would infer a subclause of $x \neq 1 \vee y \neq 1$ as a lemma, while interpolation might infer $x \neq y$ – a predicate that might be required for the inductive invariant. Spacer, that is based on this idea, is extremely effective, as demonstrated by its performance in recent CHC-COMP competitions [10]. The downside, however, is that the approach leads to a highly unstable procedure that is extremely sensitive to syntactic changes in the system description, changes in interpolation algorithms, and any algorithmic changes in the underlying SMT-solver.

An alternative approach, often called *invariant inference*, is to focus on the global safety proof, i.e., an inductive invariant. This has long been advocated by such approaches as Houdini [15], and, more recently, by a variety of machine-learning inspired techniques, e.g., FreqHorn [14], LinearArbitrary [28], and ICE-DT [16]. The key idea is to iteratively generate positive (i.e., reachable states) and negative (i.e., states that reach an error) examples and to compute a candidate invariant that separates these two sets. The reasoning is more focused towards the invariant, and, the search is restricted by either predicates, templates, grammars, or some combination. Invariant inference approaches are particularly good at finding simple inductive invariants. However, they do not generalize well to a wide variety of problems. In practice, they are often used to complement other SMT-based techniques.

In this paper, we present a novel approach that extends, what we call, *local reasoning* of IC3-style algorithms with *global guidance* inspired by the invariant inference algorithms described above. Our main insight is that the set of lemmas maintained by IC3-style algorithms hint towards a potential global proof. However, these hints are lost in existing approaches. We observe that letting the current set of lemmas, that represent candidate global invariants, guide local reasoning by introducing new lemmas and states to be blocked is often sufficient to direct IC3 towards a better global proof.

We present and implement our results in the context of Spacer—a solver for Constrained Horn Clauses (CHC)—implemented in the Z3 SMT-solver [13]. Spacer is used by multiple software model checking tools, performed remarkably well in CHC-COMP competitions [10], and is open-sourced. However, our results are fundamental and apply to any other IC3-style algorithm. While our implementation works with arbitrary CHC instances, we simplify the presentation by focusing on infinite state model checking of transition systems.

We illustrate the pitfalls of local reasoning using three examples shown in Fig. 1. All three examples are small, simple, and have simple inductive invariants.

All three are challenging for SPACER. Where these examples are based on SPACER-specific design choices, each exhibits a fundamental deficiency that stems from local reasoning. We believe they can be adapted for any other IC3-style verification algorithm. The examples assume basic familiarity with the IC3 paradigm. Readers who are not familiar with it may find it useful to read the examples after reading Sect. 2.

```
1  a, c := 0, 0;
2  // b, d := a, c;
3  b, d := 0, 0;
4  while(nd())
5  // inv: a - c = b - d;
6  {
7    if(nd()) { a++; b++; }
8    else { c++; d++; }
9  }
10 assert(a ≤ c ⇒ b ≤ d);
```

(a) myopic generalization

```
a, b := 0, 0;
while(nd())
// inv: a ≥ 0 ∧ b ≥ 0;
{
  a := a + b;
  b++;
}
assert(a ≥ 0);
```

(b) excessive generalization

```
a, b, c := 0, 0, 0;
while(nd())
// inv: b = c;
{
  a++; b++; c++;
}
assert(a ≥ 100 ⇒ b = c);
```

(c) stuck in a rut

Fig. 1. Verification tasks to illustrate sources of divergence for SPACER. The call $nd()$ non-deterministically returns a Boolean value.

Myopic Generalization. SPACER diverges on the example in Fig. 1(a) by iteratively learning lemmas of the form $(a - c \leq k) \Rightarrow (b - d \leq k)$ for different values of k, where a, b, c, d are the program variables. These lemmas establish that there are no counterexamples of longer and longer lengths. However, the process never converges to the desired lemma $(a - c) \leq (b - d)$, which excludes counterexamples of any length. The lemmas are discovered using interpolation, based on proofs found by the SMT-solver. A close examination of the corresponding proofs shows that the relationship between $(a - c)$ and $(b - d)$ does not appear in the proofs, making it impossible to find the desired lemma by tweaking local interpolation reasoning. On the other hand, looking at the global proof (i.e., the set of lemmas discovered to refute a bounded counterexample), it is almost obvious that $(a - c) \leq (b - d)$ is an interesting generalization to try. Amusingly, a small, syntactic, but semantic preserving change of swapping line 2 for line 3 in Fig. 1(a) changes the SMT-solver proofs, affects local interpolation, and makes the instance trivial for SPACER.

Excessive (Predecessor) Generalization. SPACER diverges on the example in Fig. 1(b) by computing an infinite sequence of lemmas of the form $a + k_1 \times b \geq k_2$, where a and b are program variables, and k_1 and k_2 are integers. The root cause is excessive generalization in predecessor computation. The *Bad* states are $a < 0$, and their predecessors are states such as $(a = 1 \wedge b = -10)$, $(a = 2 \wedge b = -10)$, etc., or, more generally, regions $(a + b < 0)$, $(a + 2b < -1)$, etc. SPACER always attempts to compute the most general predecessor states.

This is the best local strategy, but blocking these regions by learning their negation leads to the aforementioned lemmas. According to the global proof these lemmas do not converge to a linear invariant. An alternative strategy that under-approximates the problematic regions by (numerically) simpler regions and, as a result, learns simpler lemmas is desired (and is effective on this example). For example, region $a + 3b \leq -4$ can be under-approximated by $a \leq 32 \wedge b \leq -12$, eventually leading to a lemma $b \geq 0$, that is a part of the final invariant: $(a \geq 0 \wedge b \geq 0)$.

Stuck in a Rut. Finally, Spacer converges on the example in Fig. 1(c), but only after unrolling the system for 100 iterations. During the first 100 iterations, Spacer learns that program states with $(a \geq 100 \wedge b \neq c)$ are not reachable because a is bounded by 1 in the first iteration, by 2 in the second, and so on. In each iteration, the global proof is updated by replacing a lemma of the form $a < k$ by lemma of the form $a < (k + 1)$ for different values of k. Again, the strategy is good locally – total number of lemmas does not grow and the bounded proof is improved. Yet, globally, it is clear that no progress is made since the same set of bad states are blocked again and again in slightly different ways. An alternative strategy is to abstract the literal $a \geq 100$ from the formula that represents the bad states, and, instead, conjecture that no states in $b \neq c$ are reachable.

Our Approach: Global Guidance. As shown in the examples above, in all the cases that Spacer diverges, the missteps are not obvious locally, but are clear when the overall proof is considered. We propose three new rules, `Subsume`, `Concretize`, and, `Conjecture`, that provide global guidance, by considering existing lemmas, to mitigate the problems illustrated above. `Subsume` introduces a lemma that generalizes existing ones, `Concretize` under-approximates partially-blocked predecessors to focus on repeatedly unblocked regions, and `Conjecture` over-approximates a predecessor by abstracting away regions that are repeatedly blocked. The rules are generic, and apply to arbitrary SMT theories. Furthermore, we propose an efficient instantiation of the rules for the theory Linear Integer Arithmetic.

We have implemented the new strategy, called GSpacer, in Spacer and compared it to the original implementation of Spacer. We show that GSpacer outperforms Spacer in benchmarks from CHC-COMP 2018 and 2019. More significantly, we show that the performance is independent of interpolation. While Spacer is highly dependent on interpolation parameters, and performs poorly when interpolation is disabled, the results of GSpacer are virtually unaffected by interpolation. We also compare GSpacer to LinearArbitrary [28], a tool that *infers invariants* using global reasoning. GSpacer outperforms LinearArbitrary on the benchmarks from [28]. These results indicate that global guidance mitigates the shortcomings of local reasoning.

The rest of the paper is structured as follows. Sect. 2 presents the necessary background. Sect. 3 introduces our *global guidance* as a set of abstract inference rules. Sect. 4 describes an instantiation of the rules to Linear Integer Arithmetic

(LIA). Sect. 5 presents our empirical evaluation. Finally, Sect. 7 describes related work and concludes the paper.

2 Background

Logic. We consider first order logic modulo theories, and adopt the standard notation and terminology. A first-order language modulo theory $\mathcal{T}$ is defined over a signature Σ that consists of constant, function and predicate symbols, some of which may be *interpreted* by $\mathcal{T}$. As always, *terms* are constant symbols, variables, or function symbols applied to terms; *atoms* are predicate symbols applied to terms; *literals* are atoms or their negations; *cubes* are conjunctions of literals; and *clauses* are disjunctions of literals. Unless otherwise stated, we only consider *closed* formulas (i.e., formulas without any free variables). As usual, we use sets of formulas and their conjunctions interchangeably.

MBP. Given a set of constants $\boldsymbol{v}$, a formula φ and a model $M \models \varphi$, Model Based Projection (MBP) of φ over the constants $\boldsymbol{v}$, denoted $\text{MBP}(\boldsymbol{v}, \varphi, M)$, computes a model-preserving under-approximation of φ projected onto $\Sigma \setminus \boldsymbol{v}$. That is, $\text{MBP}(\boldsymbol{v}, \varphi, M)$ is a formula over $\Sigma \setminus \boldsymbol{v}$ such that $M \models \text{MBP}(\boldsymbol{v}, \varphi, M)$ and any model $M' \models \text{MBP}(\boldsymbol{v}, \varphi, M)$ can be extended to a model $M'' \models \varphi$ by providing an interpretation for $\boldsymbol{v}$. There are polynomial time algorithms for computing MBP in Linear Arithmetic [5,18].

Interpolation. Given an unsatisfiable formula $A \wedge B$, an interpolant, denoted $\text{ITP}(A, B)$, is a formula I over the shared signature of A and B such that $A \Rightarrow I$ and $I \Rightarrow \neg B$.

Safety Problem. A *transition system* is a pair $\langle \mathit{Init}, \mathit{Tr} \rangle$, where Init is a formula over Σ and Tr is a formula over $\Sigma \cup \Sigma'$, where $\Sigma' = \{s' \mid s \in \Sigma\}$.[1] The states of the system correspond to structures over Σ, Init represents the initial states and Tr represents the transition relation, where Σ is used to represent the pre-state of a transition, and Σ' is used to represent the post-state. For a formula φ over Σ, we denote by φ' the formula obtained by substituting each $s \in \Sigma$ by $s' \in \Sigma'$. A *safety problem* is a triple $\langle \mathit{Init}, \mathit{Tr}, \mathit{Bad} \rangle$, where $\langle \mathit{Init}, \mathit{Tr} \rangle$ is a transition system and Bad is a formula over Σ representing a set of bad states.

The safety problem $\langle \mathit{Init}, \mathit{Tr}, \mathit{Bad} \rangle$ has a *counterexample of length* k if the following formula is satisfiable: $\mathit{Init}^0 \wedge \bigwedge_{i=0}^{k-1} \mathit{Tr}^i \wedge \mathit{Bad}^k$, where φ^i is defined over $\Sigma^i = \{s^i \mid s \in \Sigma\}$ (a copy of the signature used to represent the state of the system after the execution of i steps) and is obtained from φ by substituting each $s \in \Sigma$ by $s^i \in \Sigma^i$, and Tr^i is obtained from Tr by substituting $s \in \Sigma$ by $s^i \in \Sigma^i$ and $s' \in \Sigma'$ by $s^{i+1} \in \Sigma^{i+1}$. The transition system is *safe* if the safety problem has no counterexample, of any length.

[1] In fact, a primed copy is introduced in Σ' only for the uninterpreted symbols in Σ. Interpreted symbols remain the same in Σ'.

Algorithm 1: SPACER algorithm as a set of guarded commands. We use the shorthand $\mathcal{F}(\varphi) = \mathcal{U}' \vee (\varphi \wedge Tr)$.

function SPACER:
In: $\langle Init, Tr, Bad \rangle$
Out: $\langle$SAFE, $Inv\rangle$ or UNSAFE
$Q := \emptyset$ // pob queue
$N := 0$ // maximum safe level
$\mathcal{O}_0 := Init, \mathcal{O}_i := \top$ **for all** $i > 0$ // lemma trace
$\mathcal{U} := Init$ // reachable states
forever do
Candidate $[\![$ ISSAT$(\mathcal{O}_N \wedge Bad)$ $]\!]$ $Q := Q \cup \langle Bad, N\rangle$
Predecessor $[\![$ $\langle \varphi, i+1\rangle \in Q,\ M \models \mathcal{O}_i \wedge Tr \wedge \varphi'$ $]\!]$ $Q := Q \cup \langle \text{MBP}(\boldsymbol{x}', Tr \wedge \varphi', M), i\rangle$
Successor $[\![$ $\langle \varphi, i+1\rangle \in Q,\ M \models \mathcal{F}(\mathcal{U}) \wedge \varphi'$ $]\!]$ $\mathcal{U} := \mathcal{U} \vee \text{MBP}(\boldsymbol{x}, \mathcal{F}(\mathcal{U}), M)[\boldsymbol{x}' \mapsto \boldsymbol{x}]$
Conflict $[\![$ $\langle \varphi, i+1\rangle \in Q,\ \mathcal{F}(\mathcal{O}_i) \Rightarrow \neg\varphi'$ $]\!]$ $\mathcal{O}_j := (\mathcal{O}_j \wedge \text{ITP}(\mathcal{F}(\mathcal{O}_i), \varphi')[\boldsymbol{x}' \mapsto \boldsymbol{x}])$ **for all** $j \leq i+1$
Induction $[\![$ $\ell \in \mathcal{O}_{i+1}, \ell = (\varphi \vee \psi), \mathcal{F}(\varphi \wedge \mathcal{O}_i) \Rightarrow \varphi'$ $]\!]$ $\mathcal{O}_j := \mathcal{O}_j \wedge \varphi$ **for all** $j \leq i+1$
Propagate $[\![$ $\ell \in \mathcal{O}_i, \mathcal{O}_i \wedge Tr \Rightarrow \ell'$ $]\!]$ $\mathcal{O}_{i+1} := (\mathcal{O}_{i+1} \wedge \ell)$
Unfold $[\![$ $\mathcal{O}_N \Rightarrow \neg Bad$ $]\!]$ $N := N+1$
Safe $[\![$ $\mathcal{O}_{i+1} \Rightarrow \mathcal{O}_i$ **for some** $i < N$ $]\!]$ **return** $\langle$SAFE, $\mathcal{O}_i\rangle$
Unsafe $[\![$ ISSAT$(Bad \wedge \mathcal{U})$ $]\!]$ **return** UNSAFE

Algorithm 2: Global guidance rules for SPACER.

Subsume $[\![$ $\mathcal{L} \subseteq \mathcal{O}_i, k \geq i, \mathcal{F}(\mathcal{O}_k) \Rightarrow \psi', \forall \ell \in \mathcal{L}.\, \psi \Rightarrow \ell$ $]\!]$
$\mathcal{O}_j := (\mathcal{O}_j \wedge \psi)$ **for all** $j \leq k+1$

Concretize $[\![$ $\mathcal{L} \subseteq \mathcal{O}_i, \langle \varphi, j\rangle \in Q, \forall \ell \in \mathcal{L}.$ ISSAT$(\varphi \wedge \neg\ell)$, ISSAT$(\varphi \wedge \bigwedge \mathcal{L}), \gamma \Rightarrow \varphi,$ ISSAT$(\gamma \wedge \bigwedge \mathcal{L})$ $]\!]$
$Q := Q \cup \langle \gamma, k+1\rangle$ **where** $k = \max\{j \mid \mathcal{O}_j \Rightarrow \neg\gamma\}$

Conjecture $[\![$ $\mathcal{L} \subseteq \mathcal{O}_i, \langle \varphi, j\rangle \in Q, \varphi \equiv \alpha \wedge \beta, \forall \ell \in \mathcal{L}.\, \ell \Rightarrow \neg\beta \wedge$ ISSAT$(\ell \wedge \alpha), \mathcal{U} \Rightarrow \neg\alpha$ $]\!]$
$Q := Q \cup \langle \alpha, k+1\rangle$ **where** $k = \max\{j \mid \mathcal{O}_j \Rightarrow \neg\alpha\}$

Inductive Invariants. An *inductive invariant* is a formula Inv over Σ such that (i) $Init \Rightarrow Inv$, (ii) $Inv \wedge Tr \Rightarrow Inv'$, and (iii) $Inv \Rightarrow \neg Bad$. If such an inductive invariant exists, then the transition system is safe.

Spacer. The safety problem defined above is an instance of a more general problem, CHC-SAT, of satisfiability of Constrained Horn Clauses (CHC). SPACER is a semi-decision procedure for CHC-SAT. However, to simplify the presentation, we describe the algorithm only for the particular case of the safety problem. We stress that SPACER, as well as the developments of this paper, apply to the more general setting of CHCs (both linear and non-linear). We assume that the only uninterpreted symbols in Σ are constant symbols, which we denote $\boldsymbol{x}$. Typically, these represent program variables. Without loss of generality, we assume that Bad is a cube.

Algorithm 1 presents the key ingredients of SPACER as a set of guarded commands (or rules). It maintains the following. Current unrolling depth N at which a counterexample is searched (there are no counterexamples with depth less than N). A *trace* $\mathcal{O} = (\mathcal{O}_0, \mathcal{O}_1, \ldots)$ of *frames*, such that each frame $\mathcal{O}_i$ is a set of *lemmas*, and each lemma $\ell \in \mathcal{O}_i$ is a clause. A queue of *proof obligations* Q, where each proof obligation (POB) in Q is a pair $\langle \varphi, i\rangle$ of a cube φ and a level number i, $0 \leq i \leq N$. An under-approximation $\mathcal{U}$ of reachable states. Intuitively, each frame $\mathcal{O}_i$ is a candidate inductive invariant s.t. $\mathcal{O}_i$ over-approximates states

reachable up to i steps from *Init*. The latter is ensured since $\mathcal{O}_0 = Init$, the trace is monotone, i.e., $\mathcal{O}_{i+1} \subseteq \mathcal{O}_i$, and each frame is inductive *relative* to its previous one, i.e., $\mathcal{O}_i \wedge Tr \Rightarrow \mathcal{O}'_{i+1}$. Each POB $\langle \varphi, i \rangle$ in Q corresponds to a suffix of a potential counterexample that has to be blocked in $\mathcal{O}_i$, i.e., has to be proven unreachable in i steps.

The `Candidate` rule adds an initial POB $\langle Bad, N \rangle$ to the queue. If a POB $\langle \varphi, i \rangle$ cannot be blocked because φ is reachable from frame $(i-1)$, the `Predecessor` rule generates a predecessor ψ of φ using MBP and adds $\langle \psi, i-1 \rangle$ to Q. The `Successor` rule updates the set of reachable states if the POB is reachable. If the POB is blocked, the `Conflict` rule strengthens the trace $\mathcal{O}$ by using interpolation to learn a new lemma ℓ that blocks the POB, i.e., ℓ implies $\neg\varphi$. The `Induction` rule strengthens a lemma by inductive generalization and the `Propagate` rule pushes a lemma to a higher frame. If the *Bad* state has been blocked at N, the `Unfold` rule increments the depth of unrolling N. In practice, the rules are scheduled to ensure progress towards finding a counterexample.

3 Global Guidance of Local Proofs

As illustrated by the examples in Fig. 1, while SPACER is generally effective, its local reasoning is easily confused. The effectiveness is very dependent on the local computation of predecessors using model-based projection, and lemmas using interpolation. In this section, we extend SPACER with three additional *global* reasoning rules. The rules are inspired by the deficiencies illustrated by the motivating examples in Fig. 1. In this section, we present the rules abstractly, independent of any underlying theory, focusing on pre- and post-conditions. In Sect. 4, we specialize the rules for Linear Integer Arithmetic, and show how they are scheduled with the other rules of SPACER in an efficient verification algorithm. The new global rules are summarized in Algorithm 2. We use the same guarded command notation as in description of SPACER in Algorithm 1. Note that the rules supplement, and not replace, the ones in Algorithm 1.

Subsume is the most natural rule to explain. It says that if there is a set of lemmas $\mathcal{L}$ at level i, and there exists a formula ψ such that (a) ψ is stronger than every lemma in $\mathcal{L}$, and (b) ψ over-approximates states reachable in at most k steps, where $k \geq i$, then ψ can be added to the trace to subsume $\mathcal{L}$. This rule reduces the size of the global proof – that is, the number of total not-subsumed lemmas. Note that the rule allows ψ to be at a level k that is higher than i. The choice of ψ is left open. The details are likely to be specific to the theory involved. For example, when instantiated for LIA, `Subsume` is sufficient to solve example in Fig. 1(a). Interestingly, `Subsume` is not likely to be effective for propositional IC3. In that case, ψ is a clause and the only way for it to be stronger than $\mathcal{L}$ is for ψ to be a syntactic sub-sequence of every lemma in $\mathcal{L}$, but such ψ is already explored by local inductive generalization (rule `Induction` in Algorithm 1).

Concretize applies to a POB, unlike `Subsume`. It is motivated by example in Fig. 1(b) that highlights the problem of excessive local generalization. SPACER always computes as general predecessors as possible. This is necessary for refutational completeness since in an infinite state system there are infinitely many potential predecessors. Computing the most general predecessor ensures that SPACER finds a counterexample, if it exists. However, this also forces SPACER to discover more general, and sometimes more complex, lemmas than might be necessary for an inductive invariant. Without a global view of the overall proof, it is hard to determine when the algorithm generalizes too much. The intuition for `Concretize` is that generalization is excessive when there is a single POB $\langle \varphi, j \rangle$ that is not blocked, yet, there is a set of lemmas $\mathcal{L}$ such that every lemma $\ell \in \mathcal{L}$ partially blocks φ. That is, for any $\ell \in \mathcal{L}$, there is a sub-region φ_ℓ of POB φ that is blocked by ℓ (i.e., $\ell \Rightarrow \neg\varphi_\ell$), and there is at least one state $s \in \varphi$ that is not blocked by any existing lemma in $\mathcal{L}$ (i.e., $s \models \varphi \wedge \bigwedge \mathcal{L}$). In this case, `Concretize` computes an under-approximation γ of φ that includes some not-yet-blocked state s. The new POB is added to the lowest level at which γ is not yet blocked. `Concretize` is useful to solve the example in Fig. 1(b).

Conjecture guides the algorithm away from being stuck in the same part of the search space. A single POB φ might be blocked by a different lemma at each level that φ appears in. This indicates that the lemmas are too strong, and cannot be propagated successfully to a higher level. The goal of the `Conjecture` rule is to identify such a case to guide the algorithm to explore alternative proofs with a better potential for generalization. This is done by abstracting away the part of the POB that has been blocked in the past. The pre-condition for `Conjecture` is the existence of a POB $\langle \varphi, j \rangle$ such that φ is split into two (not necessarily disjoint) sets of literals, α and β. Second, there must be a set of lemmas $\mathcal{L}$, at a (typically much lower) level $i < j$ such that every lemma $\ell \in \mathcal{L}$ blocks φ, and, moreover, blocks φ by blocking β. Intuitively, this implies that while there are many different lemmas (i.e., all lemmas in $\mathcal{L}$) that block φ at different levels, all of them correspond to a *local* generalization of $\neg\beta$ that could not be propagated to block φ at higher levels. In this case, `Conjecture` abstracts the POB φ into α, hoping to generate an alternative way to block φ. Of course, α is conjectured only if it is not already blocked and does not contain any known reachable states. `Conjecture` is necessary for a quick convergence on the example in Fig. 1(c). In some respect, `Conjecture` is akin to widening in Abstract Interpretation [12] – it abstracts a set of states by dropping constraints that appear to prevent further exploration. Of course, it is also quite different since it does not guarantee termination. While `Conjecture` is applicable to propositional IC3 as well, it is much more significant in SMT-based setting since in many FOL theories a single literal in a POB might result in infinitely many distinct lemmas.

Each of the rules can be applied by itself, but they are most effective in combination. For example, `Concretize` creates less general predecessors, that, in the worst case, lead to many simple lemmas. At the same time, `Subsume` combines lemmas together into more complex ones. The interaction of the two produces lemmas that neither one can produce in isolation. At the same time, `Conjecture`

helps unstuck the algorithm from a single unproductive POB, allowing the other rules to take effect.

4 Global Guidance for Linear Integer Arithmetic

In this section, we present a specialization of our general rules, shown in Algorithm 2, to the theory of Linear Integer Arithmetic (LIA). This requires solving two problems: identifying subsets of lemmas for pre-conditions of the rules (clearly using all possible subsets is too expensive), and applying the rule once its pre-condition is met. For lemma selection, we introduce a notion of syntactic clustering based on anti-unification. For rule application, we exploit basic properties of LIA for an effective algorithm. Our presentation is focused on LIA exclusively. However, the rules extend to combinations of LIA with other theories, such as the combined theory of LIA and Arrays.

The rest of this section is structured as follows. We begin with a brief background on LIA in Sect. 4.1. We then present our lemma selection scheme, which is common to all the rules, in Sect. 4.2, followed by a description of how the rules `Subsume` (in Sect. 4.3), `Concretize` (in Sect. 4.4), and `Conjecture` (in Sect. 4.5) are instantiated for LIA. We conclude in Sect. 4.6 with an algorithm that integrates all the rules together.

4.1 Linear Integer Arithmetic: Background

In the theory of Linear Integer Arithmetic (LIA), formulas are defined over a signature that includes interpreted function symbols $+, -, \times$, interpreted predicate symbols $<, \leq, |$, interpreted constant symbols $0, 1, 2, \ldots$, and uninterpreted constant symbols $a, b, \ldots, x, y, \ldots$. We write $\mathbb{Z}$ for the set interpreted constant symbols, and call them *integers*. We use *constants* to refer exclusively to the uninterpreted constants (these are often called *variables* in LIA literature). Terms (and accordingly formulas) in LIA are restricted to be *linear*, that is, multiplication is never applied to two constants.

We write $\text{LIA}^{-\text{div}}$ for the fragment of LIA that excludes divisiblity (d|h) predicates. A literal in $\text{LIA}^{-\text{div}}$ is a linear inequality; a cube is a conjunction of such inequalities, that is, a polytope. We find it convenient to use matrix-based notation for representing cubes in $\text{LIA}^{-\text{div}}$. A ground cube $c \in \text{LIA}^{-\text{div}}$ with p inequalities (literals) over k (uninterpreted) constants is written as $A \cdot \boldsymbol{x} \leq \boldsymbol{n}$, where A is a $p \times k$ matrix of coefficients in $\mathbb{Z}^{p \times k}$, $\boldsymbol{x} = (x_1 \cdots x_k)^T$ is a column vector that consists of the (uninterpreted) constants, and $\boldsymbol{n} = (n_1 \cdots n_p)^T$ is a column vector in $\mathbb{Z}^p$. For example, the cube $x \geq 2 \wedge 2x + y \leq 3$ is written as $\left[\begin{smallmatrix} -1 & 0 \\ 2 & 1 \end{smallmatrix}\right] \cdot \left[\begin{smallmatrix} x \\ y \end{smallmatrix}\right] \leq \left[\begin{smallmatrix} -2 \\ 3 \end{smallmatrix}\right]$. In the sequel, all vectors are column vectors, super-script T denotes transpose, dot is used for a dot product and $[\boldsymbol{n}_1; \boldsymbol{n}_2]$ stands for a matrix of column vectors $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$.

4.2 Lemma Selection

A common pre-condition for all of our global rules in Algorithm 2 is the existence of a subset of lemmas $\mathcal{L}$ of some frame $\mathcal{O}_i$. Attempting to apply the rules for every subset of $\mathcal{O}_i$ is infeasible. In practice, we use syntactic similarity between lemmas as a predictor that one of the global rules is applicable, and restrict $\mathcal{L}$ to subsets of syntactically similar lemmas. In the rest of this section, we formally define what we mean by *syntactic similarity*, and how syntactically similar subsets of lemmas, called *clusters*, are maintained efficiently throughout the algorithm.

Syntactic Similarity. A formula π with free variables is called a *pattern*. Note that we do not require π to be in LIA. Let σ be a substitution, i.e., a mapping from variables to terms. We write $\pi\sigma$ for the result of replacing all occurrences of free variables in π with their mapping under σ. A substitution σ is called *numeric* if it maps every variable to an integer, i.e., the range of σ is $\mathbb{Z}$. We say that a formula φ *numerically matches* a pattern π iff there exists a numeric substitution σ such that $\varphi = \pi\sigma$. Note that, as usual, the equality is syntactic. For example, consider the pattern $\pi = v_0 a + v_1 b \leq 0$ with free variables v_0 and v_1 and uninterpreted constants a and b. The formula $\varphi_1 = 3a + 4b \leq 0$ matches π via a numeric substitution $\sigma_1 = \{v_0 \mapsto 3, v_1 \mapsto 4\}$. However, $\varphi_2 = 4b + 3a \leq 0$, while semantically equivalent to φ_1, does not match π. Similarly $\varphi_3 = a + b \leq 0$ does not match π as well.

Matching is extended to patterns in the usual way by allowing a substitution σ to map variables to variables. We say that a pattern π_1 is more general than a pattern π_2 if π_2 matches π_1. A pattern π is a *numeric anti-unifier* for a pair of formulas φ_1 and φ_2 if both φ_1 and φ_2 match π numerically. We write $\mathit{anti}(\varphi_1, \varphi_2)$ for a most general numeric anti-unifier of φ_1 and φ_2. We say that two formulas φ_1 and φ_2 are *syntactically similar* if there exists a numeric anti-unifier between them (i.e., $\mathit{anti}(\varphi_1, \varphi_2)$ is defined). Anti-unification is extended to sets of formulas in the usual way.

Clusters. We use anti-unification to define *clusters* of syntactically similar formulas. Let Φ be a fixed set of formulas, and π a pattern. A *cluster*, $\mathcal{C}_\Phi(\pi)$, is a subset of Φ such that every formula $\varphi \in \mathcal{C}_\Phi(\pi)$ numerically matches π. That is, π is a numeric anti-unifier for $\mathcal{C}_\Phi(\pi)$. In the implementation, we restrict the pre-conditions of the global rules so that a subset of lemmas $\mathcal{L} \subseteq \mathcal{O}_i$ is a cluster for some pattern π, i.e., $\mathcal{L} = \mathcal{C}_{\mathcal{O}_i}(\pi)$.

Clustering Lemmas. We use the following strategy to efficiently keep track of available clusters. Let ℓ_{new} be a new lemma to be added to $\mathcal{O}_i$. Assume there is at least one lemma $\ell \in \mathcal{O}_i$ that numerically anti-unifies with ℓ_{new} via some pattern π. If such an ℓ does not belong to any cluster, a new cluster $\mathcal{C}_{\mathcal{O}_i}(\pi) = \{\ell_{\text{new}}, \ell\}$ is formed, where $\pi = \mathit{anti}(\ell_{\text{new}}, \ell)$. Otherwise, for every lemma $\ell \in \mathcal{O}_i$ that numerically matches ℓ_{new} and every cluster $\mathcal{C}_{\mathcal{O}_i}(\hat{\pi})$ containing ℓ, ℓ_{new} is added to $\mathcal{C}_{\mathcal{O}_i}(\hat{\pi})$ if ℓ_{new} matches $\hat{\pi}$, or a new cluster is formed using ℓ, ℓ_{new}, and any other lemmas in $\mathcal{C}_{\mathcal{O}_i}(\hat{\pi})$ that anti-unify with them. Note that a new lemma ℓ_{new} might belong to multiple clusters.

For example, suppose $\ell_{\text{new}} = (a \leq 6 \vee b \leq 6)$, and there is already a cluster $\mathcal{C}_{\mathcal{O}_i}(a \leq v_0 \vee b \leq 5) = \{(a \leq 5 \vee b \leq 5), (a \leq 8 \vee b \leq 5)\}$. Since ℓ_{new} anti-unifies with each of the lemmas in the cluster, but does not match the pattern $a \leq v_0 \vee b \leq 5$, a new cluster that includes all of them is formed w.r.t. a more general pattern: $\mathcal{C}_{\mathcal{O}_i}(a \leq v_0 \vee b \leq v_1) = \{(a \leq 6 \vee b \leq 6), (a \leq 5 \vee b \leq 5), (a \leq 8 \vee b \leq 5)\}$.

In the presentation above, we assumed that anti-unification is completely syntactic. This is problematic in practice since it significantly limits the applicability of the global rules. Recall, for example, that $a+b \leq 0$ and $2a+2b \leq 0$ do not anti-unify numerically according to our definitions, and, therefore, do not cluster together. In practice, we augment syntactic anti-unification with simple rewrite rules that are applied greedily. For example, we normalize all LIA terms, take care of implicit multiplication by 1, and of associativity and commutativity of addition. In the future, it is interesting to explore how advanced anti-unification algorithms, such as [8,27], can be adapted for our purpose.

4.3 Subsume Rule for LIA

Recall that the `Subsume` rule (Algorithm 2) takes a cluster of lemmas $\mathcal{L} = \mathcal{C}_{\mathcal{O}_i}(\pi)$ and computes a new lemma ψ that subsumes all the lemmas in $\mathcal{L}$, that is $\psi \Rightarrow \bigwedge \mathcal{L}$. We find it convenient to dualize the problem. Let $\mathcal{S} = \{\neg \ell \mid \ell \in \mathcal{L}\}$ be the dual of $\mathcal{L}$, clearly $\psi \Rightarrow \bigwedge \mathcal{L}$ iff $(\bigvee \mathcal{S}) \Rightarrow \neg\psi$. Note that $\mathcal{L}$ is a set of clauses, $\mathcal{S}$ is a set of cubes, ψ is a clause, and $\neg\psi$ is a cube. In the case of $\text{LIA}^{-\text{div}}$, this means that $\bigvee \mathcal{S}$ represents a union of convex sets, and $\neg\psi$ represents a convex set that the `Subsume` rule must find. The strongest such $\neg\psi$ in $\text{LIA}^{-\text{div}}$ exists, and is the convex closure of $\mathcal{S}$. Thus, applying `Subsume` in the context of $\text{LIA}^{-\text{div}}$ is reduced to computing a convex closure of a set of (negated) lemmas in a cluster. Full LIA extends $\text{LIA}^{-\text{div}}$ with divisibility constraints. Therefore, `Subsume` obtains a stronger $\neg\psi$ by adding such constraints.

Example 1. For example, consider the following cluster:

$$\mathcal{L} = \{(x > 2 \vee x < 2 \vee y > 3), (x > 4 \vee x < 4 \vee y > 5), (x > 8 \vee x < 8 \vee y > 9)\}$$
$$\mathcal{S} = \{(x \leq 2 \wedge x \geq 2 \wedge y \leq 3), (x \geq 4 \wedge x \leq 4 \wedge y \leq 5), (x \geq 8 \wedge x \leq 8 \wedge y \leq 9)\}$$

The convex closure of $\mathcal{S}$ in $\text{LIA}^{-\text{div}}$ is $2 \leq x \leq 8 \wedge y \leq x+1$. However, a stronger over-approximation exists in LIA: $2 \leq x \leq 8 \wedge y \leq x+1 \wedge (2 \mid x)$. □

In the sequel, we describe SUBSUMECUBE (Algorithm 3) which computes a cube φ that over-approximates $(\bigvee \mathcal{S})$. `Subsume` is then implemented by removing from $\mathcal{L}$ lemmas that are already subsumed by existing lemmas in $\mathcal{L}$, dualizing the result into $\mathcal{S}$, invoking SUBSUMECUBE on $\mathcal{S}$ and returning $\neg\varphi$ as a lemma that subsumes $\mathcal{L}$.

Recall that `Subsume` is tried only in the case $\mathcal{L} = \mathcal{C}_{\mathcal{O}_i}(\pi)$. We further require that the negated pattern, $\neg\pi$, is of the form $A \cdot \boldsymbol{x} \leq \boldsymbol{v}$, where A is a coefficients matrix, $\boldsymbol{x}$ is a vector of constants and $\boldsymbol{v} = (v_1 \cdots v_p)^T$ is a vector of p free variables. Under this assumption, $\mathcal{S}$ (the dual of $\mathcal{L}$) is of the form $\{(A \cdot \boldsymbol{x} \leq \boldsymbol{n}_i) \mid$

$1 \leq i \leq q\}$, where $q = |\mathcal{S}|$, and for each $1 \leq i \leq q$, $\boldsymbol{n}_i$ is a numeric substitution to $\boldsymbol{v}$ from which one of the negated lemmas in $\mathcal{S}$ is obtained. That is, $|\boldsymbol{n}_i| = |\boldsymbol{v}|$. In Example 1, $\neg\pi = x \leq v_1 \wedge -x \leq v_2 \wedge y \leq v_3$ and

$$A = \begin{bmatrix} 1 & 0 \\ -1 & 0 \\ 0 & 1 \end{bmatrix} \quad \boldsymbol{x} = \begin{bmatrix} x \\ y \end{bmatrix} \quad \boldsymbol{v} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} \quad \boldsymbol{n}_1 = \begin{bmatrix} 2 \\ -2 \\ 3 \end{bmatrix} \quad \boldsymbol{n}_2 = \begin{bmatrix} 4 \\ -4 \\ 5 \end{bmatrix} \quad \boldsymbol{n}_3 = \begin{bmatrix} 8 \\ -8 \\ 9 \end{bmatrix}$$

Each cube $(A \cdot \boldsymbol{x} \leq \boldsymbol{n}_i) \in \mathcal{S}$ is equivalent to $\exists \boldsymbol{v}. A \cdot \boldsymbol{x} \leq \boldsymbol{v} \wedge (\boldsymbol{v} = \boldsymbol{n}_i)$. Finally, $(\bigvee \mathcal{S}) \equiv \exists \boldsymbol{v}. (A \cdot \boldsymbol{x} \leq \boldsymbol{v}) \wedge (\bigvee (\boldsymbol{v} = \boldsymbol{n}_i))$. Thus, computing the over-approximation of $\mathcal{S}$ is reduced to (a) computing the convex hull H of a set of points $\{\boldsymbol{n}_i \mid 1 \leq i \leq q\}$, (b) computing divisibility constraints D that are satisfied by all the points, (c) substituting $H \wedge D$ for the disjunction in the equation above, and (c) eliminating variables $\boldsymbol{v}$. Both the computation of $H \wedge D$ and the elimination of $\boldsymbol{v}$ may be prohibitively expensive. We, therefore, over-approximate them. Our approach for doing so is presented in Algorithm 3, and explained in detail below.

Computing the convex hull of $\{\boldsymbol{n}_i \mid 1 \leq i \leq q\}$. lines 3 to 8 compute the convex hull of $\{\boldsymbol{n}_i \mid 1 \leq i \leq q\}$ as a formula over $\boldsymbol{v}$, where variable v_j, for $1 \leq j \leq p$, represents the j^{th} coordinates in the vectors (points) $\boldsymbol{n}_i$. Some of the coordinates, v_j, in these vectors may be linearly dependent upon others. To simplify the problem, we first identify such dependencies and compute a set of linear equalities that expresses them (L in line 4). To do so, we consider a matrix $N_{q \times p}$, where the i^{th} row consists of $\boldsymbol{n}_i^T$. The j^{th} column in N, denoted N_{*j}, corresponds to the j^{th} coordinate, v_j. The rank of N is the number of linearly independent columns (and rows). The other columns (coordinates) can be expressed by linear combinations of the linearly independent ones. To compute these linear combinations we use the kernel of $[N; \mathbf{1}]$ (N appended with a column vector of 1's), which is the set of all vectors $\boldsymbol{y}$ such that $[N; \mathbf{1}] \cdot \boldsymbol{y} = \mathbf{0}$, where $\mathbf{0}$ is the zero vector. Let $B = \text{kernel}([N; \mathbf{1}])$ be a basis for the kernel of $[N; \mathbf{1}]$. Then $|B| = p - \text{rank}(N)$, and for each vector $\boldsymbol{y} \in B$, the linear equality $[v_1 \cdots v_p \ 1] \cdot \boldsymbol{y} = 0$ holds in all the rows of N (i.e., all the given vectors satisfy it). We accumulate these equalities, which capture the linear dependencies between the coordinates, in L. Further, the equalities are used to compute $\text{rank}(N)$ coordinates (columns in N) that are linearly independent and, modulo L, uniquely determine the remaining coordinates. We denote by $\boldsymbol{v}^{L\downarrow}$ the subset of $\boldsymbol{v}$ that consists of the linearly independent coordinates. We further denote by $\boldsymbol{n}_i^{L\downarrow}$ the projection of $\boldsymbol{n}_i$ to these coordinates and by $N^{L\downarrow}$ the projection of N to the corresponding columns. We have that $(\bigvee (\boldsymbol{v} = \boldsymbol{n}_i)) \equiv L \wedge (\bigvee (\boldsymbol{v}^{L\downarrow} = \boldsymbol{n}_i^{L\downarrow}))$.

In Example 1, the numeral matrix is $N = \begin{bmatrix} 2 & -2 & 3 \\ 4 & -4 & 5 \\ 8 & -8 & 9 \end{bmatrix}$, for which $\text{kernel}([N; \mathbf{1}]) = \{(\,1\ 1\ 0\ 0\,)^T, (\,1\ 0\ -1\ 1\,)^T\}$. Therefore, L is the conjunction of equalities $v_1 + v_2 = 0 \wedge v_1 - v_3 + 1 = 0$, or, equivalently $v_3 = v_1 + 1 \wedge v_2 = -v_1$, $\boldsymbol{v}^{L\downarrow} = (v_1)^T$, and

$$\boldsymbol{n}_1^{L_\downarrow} = [2] \qquad \boldsymbol{n}_2^{L_\downarrow} = [4] \qquad \boldsymbol{n}_3^{L_\downarrow} = [8] \qquad N^{L_\downarrow} = \begin{bmatrix} 2 \\ 4 \\ 8 \end{bmatrix}$$

Next, we compute the convex closure of $\bigvee(\boldsymbol{v}^{L_\downarrow} = \boldsymbol{n}_i^{L_\downarrow})$, and conjoin it with L to obtain H, the convex closure of $(\bigvee(\boldsymbol{v} = \boldsymbol{n}_i))$.

If the dimension of $\boldsymbol{v}^{L_\downarrow}$ is one, as is the case in the example above, convex closure, C, of $\bigvee(\boldsymbol{v}^{L_\downarrow} = \boldsymbol{n}_i^{L_\downarrow})$ is obtained by bounding the sole element of $\boldsymbol{v}^{L_\downarrow}$ based on its values in $N^{L_\downarrow}$ (line 6). In Example 1, we obtain $C = 2 \leq v_1 \leq 8$.

If the dimension of $\boldsymbol{v}^{L_\downarrow}$ is greater than one, just computing the bounds of one of the constants is not sufficient. Instead, we use the concept of syntactic convex closure from [2] to compute the convex closure of $\bigvee(\boldsymbol{v}^{L_\downarrow} = \boldsymbol{n}_i^{L_\downarrow})$ as $\exists \boldsymbol{\alpha}. C$ where $\boldsymbol{\alpha}$ is a vector that consists of q fresh *rational* variables and C is defined as follows (line 8): $C = \boldsymbol{\alpha} \geq 0 \wedge \Sigma\boldsymbol{\alpha} = 1 \wedge \boldsymbol{\alpha}^T \cdot N^{L_\downarrow} = (\boldsymbol{v}^{L_\downarrow})^T$. C states that $(\boldsymbol{v}^{L_\downarrow})^T$ is a convex combination of the rows of $N^{L_\downarrow}$, or, in other words, $\boldsymbol{v}^{L_\downarrow}$ is a convex combination of $\{\boldsymbol{n}_i^{L_\downarrow} \mid 1 \leq i \leq q\}$.

To illustrate the syntactic convex closure, consider a second example with a set of cubes: $\mathcal{S} = \{(x \leq 0 \wedge y \leq 6), (x \leq 6 \wedge y \leq 0), (x \leq 5 \wedge y \leq 5)\}$. The coefficient matrix A, and the numeral matrix N are then: $A = \left[\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right]$ and $N = \left[\begin{smallmatrix} 0 & 6 \\ 6 & 0 \\ 5 & 5 \end{smallmatrix}\right]$. Here, kernel($[N; \mathbf{1}]$) is empty – all the columns are linearly independent, hence, $L = \mathit{true}$ and $\boldsymbol{v}^{L_\downarrow} = \boldsymbol{v}$. Therefore, syntactic convex closure is applied to the full matrix N, resulting in

$$C = (\alpha_1 \geq 0) \wedge (\alpha_2 \geq 0) \wedge (\alpha_3 \geq 0) \wedge (\alpha_1 + \alpha_2 + \alpha_3 = 1) \wedge \\ (6\alpha_2 + 5\alpha_3 = v_1) \wedge (6\alpha_1 + 5\alpha_3 = v_2)$$

The convex closure of $\bigvee(\boldsymbol{v} = \boldsymbol{n}_i)$ is then $L \wedge \exists \boldsymbol{\alpha}. C$, which is $\exists \boldsymbol{\alpha}. C$ here.

Divisibility Constraints. Inductive invariants for verification problems often require divisibility constraints. We, therefore, use such constraints, denoted D, to obtain a stronger over-approximation of $\bigvee(\boldsymbol{v} = \boldsymbol{n}_i)$ than the convex closure. To add a divisibility constraint for $v_j \in \boldsymbol{v}^{L_\downarrow}$, we consider the column $N_{*j}^{L_\downarrow}$ that corresponds to v_j in $N^{L_\downarrow}$. We find the largest positive integer d such that each integer in $N_{*j}^{L_\downarrow}$ leaves the same remainder when divided by d; namely, there exists $0 \leq r < d$ such that $n \bmod d = r$ for every $n \in N_{*j}^{L_\downarrow}$. This means that $d \mid (v_j - r)$ is satisfied by all the points $\boldsymbol{n}_i$. Note that such r always exists for $d = 1$. To avoid this trivial case, we add the constraint $d \mid (v_j - r)$ only if $d \neq 1$ (line 12). We repeat this process for each $v_j \in \boldsymbol{v}^{L_\downarrow}$.

In Example 1, all the elements in the (only) column of the matrix $N^{L_\downarrow}$, which corresponds to v_1, are divisible by 2, and no larger d has a corresponding r. Thus, line 12 of Algorithm 3 adds the divisibility condition $(2 \mid v_1)$ to D.

Eliminating Existentially Quantified Variables Using MBP. By combining the linear equalities exhibited by N, the convex closure of $N^{L_\downarrow}$ and the divisibility constraints on $\boldsymbol{v}$, we obtain $\exists \boldsymbol{\alpha}.\, L \wedge C \wedge D$ as an over-approximation of $\bigvee(\boldsymbol{v} = \boldsymbol{n}_i)$. Accordingly, $\exists \boldsymbol{v}.\, \exists \boldsymbol{\alpha}.\, \psi$, where $\psi = (A \cdot \boldsymbol{x} \leq \boldsymbol{v}) \wedge L \wedge C \wedge D$, is an over-approximation of $(\bigvee \mathcal{S}) \equiv \exists \boldsymbol{v}.\, (A \cdot \boldsymbol{x} \leq \boldsymbol{v}) \wedge (\bigvee(\boldsymbol{v} = \boldsymbol{n}_i))$ (line 13). In order to get a LIA cube that overapproximates $\bigvee \mathcal{S}$, it remains to eliminate the existential quantifiers. Since quantifier elimination is expensive, and does not necessarily generate convex formulas (cubes), we approximate it using MBP. Namely, we obtain a cube φ that under-approximates $\exists \boldsymbol{v}.\, \exists \boldsymbol{\alpha}.\, \psi$ by applying MBP on ψ and a model $M_0 \models \psi$. We then use an SMT solver to drop literals from φ until it over-approximates $\exists \boldsymbol{v}.\, \exists \boldsymbol{\alpha}.\, \psi$, and hence also $\bigvee \mathcal{S}$ (lines 16 to 19). The result is returned by `Subsume` as an over-approximation of $\bigvee \mathcal{S}$.

Models M_0 that satisfy ψ and do not satisfy any of the cubes in $\mathcal{S}$ are preferred when computing MBP (line 14) as they ensure that the result of MBP is not subsumed by any of the cubes in $\mathcal{S}$.

Note that the $\boldsymbol{\alpha}$ are rational variables and $\boldsymbol{v}$ are integer variables, which means we require MBP to support a mixture of integer and rational variables. To achieve this, we first relax all constants to be rationals and apply MBP over LRA to eliminate $\boldsymbol{\alpha}$. We then adjust the resulting formula back to integer arithmetic by multiplying each atom by the least common multiple of the denominators of the coefficients in it. Finally, we apply MBP over the integers to eliminate $\boldsymbol{v}$.

Considering Example 1 again, we get that $\psi = (x \leq v_1) \wedge (-x \leq v_2) \wedge (y \leq v_3) \wedge (v_3 = 1 + v_1) \wedge (v_2 = -v_1) \wedge (2 \leq v_1 \leq 8) \wedge (2 \mid v_1)$ (the first three conjuncts correspond to $(A \cdot (x\ y)^T \leq (v_1\ v_2\ v_3)^T)$). Note that in this case we do not have rational variables $\boldsymbol{\alpha}$ since $|\boldsymbol{v}^{L_\downarrow}| = 1$. Depending on the model, the result of MBP can be one of

$$y \leq x + 1 \wedge 2 \leq x \leq 8 \wedge (2 \mid y - 1) \wedge (2 \mid x) \qquad x \geq 2 \wedge x \leq 2 \wedge y \leq 3$$
$$y \leq x + 1 \wedge 2 \leq x \leq 8 \wedge (2 \mid x) \qquad x \geq 8 \wedge x \leq 8 \wedge y \leq 9$$
$$y \geq x + 1 \wedge y \leq x + 1 \wedge 3 \leq y \leq 9 \wedge (2 \mid y - 1)$$

However, we prefer a model that does not satisfy any cube in $\mathcal{S} = \{(x \geq 2 \wedge x \leq 2 \wedge y \leq 3), (x \leq 4 \wedge x \geq 4 \wedge y \leq 5), (x \leq 8 \wedge x \geq 8 \wedge y \leq 9)\}$, rules off the two possibilities on the right. None of these cubes cover ψ, hence generalization is used.

If the first cube is obtained by MBP, it is generalized into $y \leq x + 1 \wedge x \geq 2 \wedge x \leq 8 \wedge (2|x)$; the second cube is already an over-approximation; the third cube is generalized into $y \leq x + 1 \wedge y \leq 9$. Indeed, each of these cubes over-approximates $\bigvee \mathcal{S}$.

4.4 Concretize Rule for LIA

The `Concretize` rule (Algorithm 2) takes a cluster of lemmas $\mathcal{L} = \mathcal{C}_{\mathcal{O}_i}(\pi)$ and a POB $\langle \varphi, j \rangle$ such that each lemma in $\mathcal{L}$ partially blocks φ, and creates a new POB γ that is still not blocked by $\mathcal{L}$, but γ is more concrete, i.e., $\gamma \Rightarrow \varphi$. In our implementation, this rule is applied when φ is in $\text{LIA}^{-\text{div}}$. We further require that the pattern, π, of $\mathcal{L}$ is non-linear, i.e., some of the constants appear in π with free variables

Algorithm 3: An implementation of the Subsume rule for the dual of a cluster $\mathcal{S} = \{A \cdot \boldsymbol{x} \leq \boldsymbol{n}_i \mid 1 \leq i \leq q\}$.

1 **function** subsumeCube:
  In: $\mathcal{S} = \{(A \cdot \boldsymbol{x} \leq \boldsymbol{n}_i) \mid 1 \leq i \leq q\}$,
  Out: An over-approximation of $(\bigvee \mathcal{S})$.
  /* $\boldsymbol{v}$ are integer variables such that:
    $(\bigvee \mathcal{S}) \iff \exists \boldsymbol{v}. (A \cdot \boldsymbol{x} \leq \boldsymbol{v}) \wedge (\bigvee \boldsymbol{v} = \boldsymbol{n}_i)$ */
2 $N := [\boldsymbol{n}_1; \cdots; \boldsymbol{n}_q]^T$
  /* Compute the set of linear dependencies implied by N */
3 $B := \text{kernel}([N; \mathbf{1}])$
4 $L := \bigwedge_{y \in B} (v_1 \cdots v_p\ 1) \cdot \boldsymbol{y} = 0$
5 **if** $|\boldsymbol{v}^{L\downarrow}| = 1$ **then**
    // Convex closure over a single constant $v_i \in \boldsymbol{v}^{L\downarrow}$
6 $C := \min(N_{*i}) \leq v_i \leq \max(N_{*i})$
7 **else**
    // Syntactic convex closure
8 $C := (\boldsymbol{\alpha}^T \cdot N^{L\downarrow} = (\boldsymbol{v}^{L\downarrow})^T) \wedge (\Sigma \boldsymbol{\alpha} = 1) \wedge (\boldsymbol{\alpha} \geq 0)$
  /* Compute divisibility constraints */
9 $D := \top$
10 **for** $v_j \in \boldsymbol{v}^{L\downarrow}$ **do**
11 **if** $\exists d, r.\, d \neq 1 \wedge (\forall n \in N_{*j}^{L\downarrow}. (n \bmod d = r))$ **then**
12 $D := D \wedge d \mid (v_j - r)$
13 $\psi := (A \cdot \boldsymbol{x} \leq \boldsymbol{v}) \wedge L \wedge C \wedge D$
  /* Under-approximate quantifier elimination */
14 find M_0 s.t. $M_0 \models \psi$ and, if possible, $M_0 \not\models (\bigvee S)$
15 $\varphi := \text{MBP}((\boldsymbol{\alpha}\ \boldsymbol{v}), \psi, M_0)$
  /* Over-approximate quantifier elimination */
16 **while** isSat$(\neg\varphi \wedge \psi)$ **do**
17 find M_1 s.t. $M_1 \models (\neg\varphi \wedge \psi)$
18 $\varphi := \bigwedge \{\ell \in \varphi \mid \neg(M_1 \models \neg\ell)\}$
19 **return** φ

Algorithm 4: An implementation of the Concretize rule in LIA.

1 **function** Concretize:
  In: A pob $\langle \varphi, j \rangle$ in LIA$^{-\text{div}}$, a cluster of LIA$^{-\text{div}}$ lemmas $\mathcal{L} = \mathcal{C}_{\mathcal{O}_j}(\pi)$ s.t. π is non-linear, isSat$(\varphi \wedge \bigwedge \mathcal{L})$
  Out: A cube γ such that $\gamma \Rightarrow \varphi$ and $\forall \ell \in \mathcal{L}.$ isSat$(\gamma \wedge \ell)$
2 $U := \{x \mid \text{coeff}(x, \pi) \in \text{Vars}(\pi)\}$
3 find M s.t. $M \models \varphi \wedge \bigwedge \mathcal{L}$
4 $\gamma := \top$
5 **foreach** $lit \in \varphi$ **do**
6 **if** Consts$(lit) \cap U \neq \emptyset$ **then**
    $\gamma := \gamma \wedge$ Concretize_lit(lit, M, U)
7 **else** $\gamma := \gamma \wedge lit$
8 $\gamma :=$ rm_subsume(γ)
9 **return** γ
10 **function** Concretize_lit:
  In: A literal $lit = \Sigma_i n_i x_i \leq b_j$ in LIA$^{-\text{div}}$, model $M \models lit$, and a set of constants U
  Out: A cube γ^{lit} that concretizes lit
  /* Construct a single literal using all the constants in Consts$(lit) \setminus U$ */
11 $\gamma^{lit} := \emptyset$
12 $s := 0$
13 **foreach** $x_i \in$ Consts$(lit) \setminus U$ **do**
14 $s := s + n_i x_i$
15 $\gamma^{lit} := (s \leq M[s])$
  /* Generate one dimensional literals for each constant in U */
16 **foreach** $x_i \in$ Consts$(lit) \cap U$ **do**
17 $\gamma^{lit} := \gamma^{lit} \wedge (n_i x_i \leq M[n_i x_i])$
18 **return** γ^{lit}

as their coefficients. We denote these constants by U. An example is the pattern $\pi = v_0 x + v_1 y + z \leq 0$, where $U = \{x, y\}$. Having such a cluster is an indication that attempting to block φ in full with a single lemma may require to track non-linear correlations between the constants, which is impossible to do in LIA. In such cases, we identify the coupling of the constants in U in pobs (and hence in lemmas) as the potential source of non-linearity. Hence, we concretize (strengthen) φ into a pob γ where the constants in U are no longer coupled to any other constant.

Coupling. Formally, constants u and v are *coupled* in a cube c, denoted $u \bowtie_c v$, if there exists a literal *lit* in c such that both u and v appear in *lit* (i.e., their coefficients in *lit* are non-zero). For example, x and y are coupled in $x + y \leq 0 \wedge z \leq 0$ whereas neither of them are coupled with z. A constant u is said to be *isolated* in a cube c, denoted Iso(u, c), if it appears in c but it is not coupled with any other constant in c. In the above cube, z is isolated.

Concretization by Decoupling. Given a pob φ (a cube) and a cluster $\mathcal{L}$, Algorithm 4 presents our approach for concretizing φ by decoupling the constants in U—those that have variables as coefficients in the pattern of $\mathcal{L}$ (line 2). Concretization is guided by a model $M \models \varphi \wedge \bigwedge \mathcal{L}$, representing a part of φ that is not yet blocked by the lemmas in $\mathcal{L}$ (line 3). Given such M, we concretize φ

into a *model-preserving* under-approximation that isolates all the constants in U and preserves all other couplings. That is, we find a cube γ, such that

$$\gamma \Rightarrow \varphi \quad M \models \gamma \quad \forall u \in U.\, \textsc{Iso}(u, \gamma) \quad \forall u, v \notin U.\, (u \bowtie_\varphi v) \Rightarrow (u \bowtie_\gamma v) \tag{1}$$

Note that γ is not blocked by $\mathcal{L}$ since M satisfies both $\bigwedge \mathcal{L}$ and γ. For example, if $\varphi = (x+y \leq 0) \wedge (x-y \leq 0) \wedge (x+z \geq 0)$ and $M = [x = 0, y = 0, z = 1]$, then $\gamma = 0 \leq y \leq 0 \wedge x \leq 0 \wedge x + z \geq 1$ is a model preserving under-approximation that isolates $U = \{y\}$.

Algorithm 4 computes such a cube γ by a point-wise concretization of the literals of φ followed by the removal of subsumed literals. Literals that do not contain constants from U remain unchanged. A literal of the form $lit = t \leq b$, where $t = \sum_i n_i x_i$ (recall that every literal in $\text{LIA}^{-\text{div}}$ can be normalized to this form), that includes constants from U is concretized into a *cube* by (1) isolating each of the summands $n_i x_i$ in t that include U from the rest, and (2) for each of the resulting sub-expressions creating a literal that uses its value in M as a bound. Formally, t is decomposed to $s + \sum_{x_i \in U} n_i x_i$, where $s = \sum_{x_i \notin U} n_i x_i$. The concretization of lit is the cube $\gamma^{lit} = s \leq M[s] \wedge \bigwedge_{x_i \in U} n_i x_i \leq M[n_i x_i]$, where $M[t']$ denotes the interpretation of t' in M. Note that $\gamma^{lit} \Rightarrow lit$ since the bounds are stronger than the original bound on t: $M[s] + \sum_{x_i \in U} M[n_i x_i] = M[t] \leq b$. This ensures that γ, obtained by the conjunction of literal concretizations, implies φ. It trivially satisfies the other conditions of Eq. (1).

For example, the concretization of the literal $(x + y \leq 0)$ with respect to $U = \{y\}$ and $M = [x = 0, y = 0, z = 1]$ is the cube $x \leq 0 \wedge y \leq 0$. Applying concretization in a similar manner to all the literals of the cube $\varphi = (x+y \leq 0) \wedge (x-y \leq 0) \wedge (x+z \geq 0)$ from the previous example, we obtain the concretization $x \leq 0 \wedge 0 \leq y \leq 0 \wedge x + z \geq 0$. Note that the last literal is not concretized as it does not include y.

4.5 Conjecture Rule for LIA

The `Conjecture` rule (see Algorithm 2) takes a set of lemmas $\mathcal{L}$ and a POB $\varphi \equiv \alpha \wedge \beta$ such that all lemmas in $\mathcal{L}$ block β, but none of them blocks α, where α does not include any known reachable states. It returns α as a new POB.

For LIA, `Conjecture` is applied when the following conditions are met: (1) the POB φ is of the form $\varphi_1 \wedge \varphi_2 \wedge \varphi_3$, where $\varphi_3 = (\boldsymbol{n}^T \cdot \boldsymbol{x} \leq b)$, and φ_1 and φ_2 are any cubes. The sub-cube $\varphi_1 \wedge \varphi_2$ acts as α, while the sub-cube $\varphi_2 \wedge \varphi_3$ acts as β. (2) The cluster $\mathcal{L}$ consists of $\{bg \vee (\boldsymbol{n}^T \cdot \boldsymbol{x} \geq b_i) \mid 1 \leq i \leq q\}$, where $b_i > b$ and $bg \Rightarrow \neg\varphi_2$. This means that each of the lemmas in $\mathcal{L}$ blocks $\beta = \varphi_2 \wedge \varphi_3$, and they may be ordered as a sequence of increasingly stronger lemmas, indicating that they were created by trying to block the POB at different levels, leading to too strong lemmas that failed to propagate to higher levels. (3) The formula $(bg \vee (\boldsymbol{n}^T \cdot \boldsymbol{x} \geq b_i)) \wedge \varphi_1 \wedge \varphi_2$ is satisfiable, that is, none of the lemmas in $\mathcal{L}$ block $\alpha = \varphi_1 \wedge \varphi_2$, and (4) $\mathcal{U} \Rightarrow \neg(\varphi_1 \wedge \varphi_2)$, that is, no state in $\varphi_1 \wedge \varphi_2$ is known to be reachable. If all four conditions are met, we conjecture $\alpha = \varphi_1 \wedge \varphi_2$. This is implemented by CONJECTURE, that returns α (or $\bot$ when the pre-conditions are not met).

Algorithm 5: GSpacer for LIA.

```
1  function GSpacer:
   In: ⟨Init, Tr, Bad⟩
   Out: An Inductive invariant or UNSAFE
   /* Initialize state of the solver */
2  Q := ∅; N := 0; U := Init;
3  O_0 := Init; O_i := ⊤, ∀i > 0
4  Enqueue(Q, ⟨Bad, 0⟩)
5  while ⊤ do
6    ⟨φ, i⟩ := Pop(Q)
7    if ConcretizePOB(⟨φ, i⟩) = ⊤ then
8      continue
9    if isSat(F(O_{i−1}) ∧ φ′) then
       // The pob φ cannot be blocked at i
10     AddPredecessor(⟨φ, i⟩)
11     if isSat(U ∧ Bad) then
12       return UNSAFE                          // Unsafe
13   else
       // The pob φ can be blocked at i
14     Block(⟨φ, i⟩)
15     for 0 ≤ j ≤ N do
16       for ℓ ∈ O_j \ O_{j+1} do
17         if O_j ∧ Tr ⇒ ℓ′ then
18           O_{j+1} := O_{j+1} ∧ ℓ              // Propagate
19     if ∃0 ≤ j < N · O_j ⇒ O_{j−1} then
20       return ⟨SAFE, O_j⟩                     // Safe
21     if O_N ⇒ ¬Bad then
22       N := N + 1                             // Unfold
23     push(Q, ⟨Bad, N⟩)

24 function ConcretizePOB:
25   ⟨π_1, L_1⟩ := C_pob(⟨φ, i⟩)
26   L_2 := {ℓ | ℓ ∈ L_1 ∧ isSat(ℓ ∧ φ) ∧ isSat(¬ℓ ∧ φ)}
27   if (L_2 ≠ ∅ ∧ nonLin(π_1) ∧ isSat(⋀ L_2 ∧ φ)) then
28     γ := Concretize(φ, ⟨π_1, L_2⟩)
29     k := max{j | O_j ⇒ ¬γ}
30     push(Q, ⟨γ, k⟩)                          // Concretize
31     push(Q, ⟨φ, i⟩)
32     return ⊤
33   else return ⊥

34 function AddPredecessor:
35   if isSat(F(U) ∧ φ′) then
36     find M_1 s.t M_1 ⊨ F(U) ∧ φ′
37     s := (MBP(x, F(U), M_1)[x′ ↦ x])
38     U := U ∨ s                               // Successor
39     return
40   find M_2 s.t M_2 ⊨ Θ
41   p := MBP(x′, Tr ∧ φ′, M_2)
42   push(Q, ⟨p, i − 1⟩)                        // Predecessor
43   push(Q, ⟨φ, i⟩)

44 function Block:
45   ℓ := GEN(F(O_{i−1}), φ′)                   // Conflict
46   for 0 ≤ j ≤ i do O_j := O_j ∧ ℓ
47   ⟨π_3, L_3⟩ = C_lemma(ℓ)
48   α := Conjecture(φ, L_3, U)
49   if α ≠ ⊥ then
50     k := max{j | O_j ⇒ ¬α}
51     push(Q, ⟨α, k⟩)                          // Conjecture
52   if ¬π_3 = A · x ≤ v then
53     ψ := subsume(⟨π_3, L_3⟩)
54     k := max{j | F(O_j) ⇒ ψ′}
55     O_j := O_j ∧ ψ for all j ≤ k + 1          // Subsume
```

For example, consider the POB $\varphi = x \geq 10 \wedge (x + y \geq 10) \wedge y \leq 10$ and a cluster of lemmas $\mathcal{L} = \{(x + y \leq 0 \vee y \geq 101), (x + y \leq 0 \vee y \geq 102)\}$. In this case, $\varphi_1 = x \geq 10$, $\varphi_2 = (x + y \geq 10)$, $\varphi_3 = y \leq 10$, and $bg = x + y \leq 0$. Each of the lemmas in $\mathcal{L}$ block $\varphi_2 \wedge \varphi_3$ but none of them block $\varphi_1 \wedge \varphi_2$. Therefore, we conjecture $\varphi_1 \wedge \varphi_2$: $x \geq 10 \wedge (x + y \geq 10)$.

4.6 Putting It All Together

Having explained the implementation of the new rules for LIA, we now put all the ingredients together into an algorithm, GSpacer. In particular, we present our choices as to when to apply the new rules, and on which clusters of lemmas and POBs. As can be seen in Sect. 5, this implementation works very well on a wide range of benchmarks.

Algorithm 5 presents GSpacer. The comments to the right side of a line refer to the abstract rules in Algorithm 1 and 2. Just like Spacer, GSpacer iteratively computes predecessors (line 10) and blocks them (line 14) in an infinite loop. Whenever a POB is proven to be reachable, the reachable states are updated (line 38). If *Bad* intersects with a reachable state, GSpacer terminates and returns UNSAFE (line 12). If one of the frames is an inductive invariant, GSpacer terminates with SAFE (line 20).

When a POB $\langle \varphi, i \rangle$ is handled, we first apply the `Concretize` rule, if possible (line 7). Recall that Concretize (Algorithm 4) takes as input a cluster that

partially blocks φ and has a non-linear pattern. To obtain such a cluster, we first find, using $\mathcal{C}_{pob}(\langle\varphi, i\rangle)$, a cluster $\langle\pi_1, \mathcal{L}_1\rangle = \mathcal{C}_{\mathcal{O}_k}(\pi_1)$, where $k \leq i$, that includes *some* lemma (from frame k) that blocks φ; if none exists, $\mathcal{L}_1 = \emptyset$. We then filter out from $\mathcal{L}_1$ lemmas that completely block φ as well as lemmas that are irrelevant to φ, i.e., we obtain $\mathcal{L}_2$ by keeping only lemmas that partially block φ. We apply Concretize on $\langle\pi_1, \mathcal{L}_2\rangle$ to obtain a new pob that under-approximates φ if (1) the remaining sub-cluster, $\mathcal{L}_2$, is non-empty, (2) the pattern, π_1, is non-linear, and (3) $\bigwedge \mathcal{L}_2 \wedge \varphi$ is satisfiable, i.e., a part of φ is not blocked by any lemma in $\mathcal{L}_2$.

Once a pob is blocked, and a new lemma that blocks it, ℓ, is added to the frames, an attempt is made to apply the `Subsume` and `Conjecture` rules on a cluster that includes ℓ. To that end, the function $\mathcal{C}_{lemma}(\ell)$ finds *a* cluster $\langle\pi_3, \mathcal{L}_3\rangle = \mathcal{C}_{\mathcal{O}_i}(\pi_3)$ to which ℓ belongs (Sect. 4.2). Note that the choice of cluster is arbitrary. The rules are applied on $\langle\pi_3, \mathcal{L}_3\rangle$ if the required pre-conditions are met (line 49 and line 53, respectively). When applicable, Subsume returns a new lemma that is added to the frames, while Conjecture returns a new pob that is added to the queue. Note that the latter is a *may* pob, in the sense that some of the states it represents *may not* lead to safety violation.

Ensuring Progress. Spacer always makes progress: as its search continues, it establishes absence of counterexamples of deeper and deeper depths. However, GSpacer does not ensure progress. Specifically, unrestricted application of the `Concretize` and `Conjecture` rules can make GSpacer diverge even on executions of a fixed bound. In our implementation, we ensure progress by allotting a fixed amount of *gas* to each pattern, π, that forms a cluster. Each time `Concretize` or `Conjecture` is applied to a cluster with π as the pattern, π loses some gas. Whenever π runs out of gas, the rules are no longer applied to any cluster with π as the pattern. There are finitely many patterns (assuming LIA terms are normalized). Thus, in each bounded execution of GSpacer, the `Concretize` and `Conjecture` rules are applied only a finite number of times, thereby, ensuring progress. Since the `Subsume` rule does not hinder progress, it is applied without any restriction on gas.

5 Evaluation

We have implemented[2] GSpacer (Algorithm 5) as an extension to Spacer. To reduce the dimension of a matrix (in subsume, Sect. 4.3), we compute pairwise linear dependencies between all pairs of columns instead of computing the full kernel. This does not necessarily reduce the dimension of the matrix to its rank, but, is sufficient for our benchmarks. We have experimented with computing the full kernel using SageMath [25], but the overall performance did not improve. Clustering is implemented by anti-unification. LIA terms are normalized using

[2] https://github.com/hgvk94/z3/tree/gspacer-cav-ae.

default Z3 simplifications. Our implementation also supports global generalization for non-linear CHCs. We have also extended our work to the theory of LRA. We defer the details of this extension to an extended version of the paper.

To evaluate our implementation, we have conducted two sets of experiments[3]. All experiments were run on Intel E5-2690 V2 CPU at 3 GHz with 128 GB memory with a timeout of 10 min. First, to evaluate the performance of local reasoning with global guidance against pure local reasoning, we have compared GSpacer with the latest Spacer, to which we refer as the *baseline*. We took the benchmarks from CHC-COMP 2018 and 2019 [10]. We compare to Spacer because it dominated the competition by solving 85% of the benchmarks in CHC-COMP 2019 (20% more than the runner up) and 60% of the benchmarks in CHC-COMP 2018 (10% more than runner up). Our evaluation shows that GSpacer outperforms Spacer both in terms of number of solved instances and, more importantly, in overall robustness.

Second, to examine the performance of local reasoning with global guidance compared to solely global reasoning, we have compared GSpacer with an ML-based data-driven invariant inference tool LinearArbitrary [28]. Compared to other similar approaches, LinearArbitrary stands out by supporting invariants with arbitrary Boolean structure over arbitrary linear predicates. It is completely automated and does not require user-provided predicates, grammars, or any other guidance. For the comparison with LinearArbitrary, we have used both the CHC-COMP benchmarks, as well as the benchmarks from the artifact evaluation of [28]. The machine and timeout remain the same. Our evaluation shows that GSpacer is superior in this case as well.

Comparison with Spacer. Table 1 summarizes the comparison between Spacer and GSpacer on CHC-COMP instances. Since both tools can use a variety of interpolation strategies during lemma generalization (Line 45 in Algorithm 5), we compare three different configurations of each: *bw* and *fw* stand for two interpolation strategies, *backward* and *forward*, respectively, already implemented in Spacer, and *sc* stands for turning interpolation off and generalizing lemmas only by *subset clauses* computed by inductive generalization.

Any configuration of GSpacer solves significantly more instances than even the best configuration of Spacer. Figure 2 provides a more detailed comparison between the best configurations of both tools in terms of running time and depth of convergence. There is no clear trend in terms of running time on instances solved by both tools. This is not surprising—SMT-solving run time is highly non-deterministic and any change in strategy has a significant impact on performance of SMT queries involved. In terms of depth, it is clear that GSpacer converges at the same or lower depth. The depth is significantly lower for instances solved only by GSpacer.

Moreover, the performance of GSpacer is not significantly affected by the interpolation strategy used. In fact, the configuration *sc* in which interpolation is

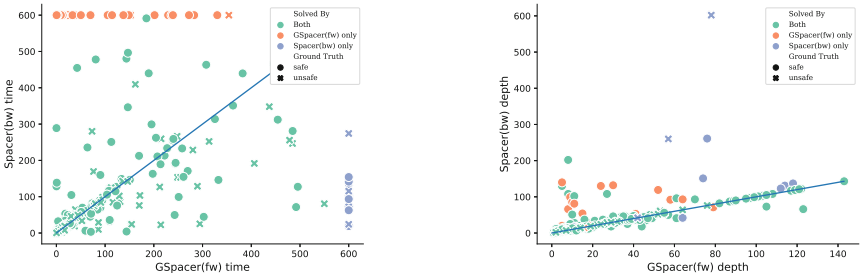
[3] Detailed experimental results including the effectiveness of each rule, and the extensions to non-linear CHCs and LRA can be found at https://hgvk94.github.io/gspacer/.

disabled performs the best in CHC-COMP 2018, and only slightly worse in CHC-COMP 2019! In comparison, disabling interpolation hurts SPACER significantly.

Figure 3 provides a detailed comparison of GSPACER with and without interpolation. Interpolation makes no difference to the depth of convergence. This implies that lemmas that are discovered by interpolation are discovered as efficiently by the global rules of GSPACER. On the other hand, interpolation significantly increases the running time. Interestingly, the time spent in interpolation itself is insignificant. However, the lemmas produced by interpolation tend to slow down other aspects of the algorithm. Most of the slow down is in increased time for inductive generalization and in computation of predecessors. The comparison between the other interpolation-enabled strategy and GSPACER (*sc*) shows a similar trend.

Table 1. Comparison between SPACER and GSPACER on CHC-COMP.

Bench	SPACER						GSPACER							
	fw		bw		sc		fw		bw		sc		VBS	
	safe	unsafe	safe	unsafe	safe	unsafe	safe	unsafe	safe	unsafe	safe	unsafe	safe	unsafe
CHC-18	159	66	163	**69**	123	68	**214**	67	**214**	63	**214**	**69**	229	74
CHC-19	193	84	186	84	125	84	**202**	84	196	**85**	200	84	207	85

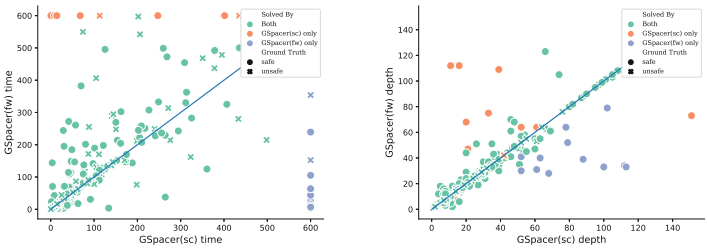


(a) running time (b) depth explored

Fig. 2. Best configurations: GSPACER versus SPACER.

Comparison with LINEARARBITRARY. In [28], the authors show that LINEARARBITRARY, to which we refer as LARB for short, significantly outperforms SPACER on a curated subset of benchmarks from SV-COMP [24] competition.

At first, we attempted to compare LARB against GSPACER on the CHC-COMP benchmarks. However, LARB did not perform well on them. Even the



(a) running time (b) depth explored

Fig. 3. Comparing GSpacer with different interpolation tactics.

baseline Spacer has outperformed LArb significantly. Therefore, for a more meaningful comparison, we have also compared Spacer, LArb and GSpacer on the benchmarks from the artifact evaluation of [28]. The results are summarized in Table 2. As expected, LArb outperforms the baseline Spacer on the safe benchmarks. On unsafe benchmarks, Spacer is significantly better than LArb. In both categories, GSpacer dominates solving more safe benchmarks than either Spacer or LArb, while matching performance of Spacer on unsafe instances. Furthermore, GSpacer remains orders of magnitude faster than LArb on benchmarks that are solved by both. This comparison shows that incorporating local reasoning with global guidance not only mitigates its shortcomings but also surpasses global data-driven reasoning.

Table 2. Comparison with LArb.

Bench	Spacer		LArb		GSpacer		VB	
	safe	unsafe	safe	unsafe	safe	unsafe	safe	unsafe
PLDI18	216	**68**	270	65	**279**	**68**	284	68

6 Related Work

The limitations of local reasoning in SMT-based infinite state model checking are well known. Most commonly, they are addressed with either (a) different strategies for local generalization in interpolation (e.g., [1,6,19,23]), or (b) shifting the focus to *global* invariant inference by learning an invariant of a restricted shape (e.g., [9,14–16,28]).

Interpolation Strategies. Albarghouthi and McMillan [1] suggest to minimize the number of literals in an interpolant, arguing that simpler (i.e., fewer half-spaces) interpolants are more likely to generalize. This helps with myopic generalizations (Fig. 1(a)), but not with excessive generalizations (Fig. 1(b)). On the contrary,

Blicha et al. [6] decompose interpolants to be numerically simpler (but with more literals), which helps with excessive, but not with myopic, generalizations. Deciding *locally* between these two techniques or on their combination (i.e., some parts of an interpolant might need to be split while others combined) seems impossible. Schindler and Jovanovic [23] propose local interpolation that bounds the number of lemmas generated from a single POB (which helps with Fig. 1(c)), but only if inductive generalization is disabled. Finally, [19] suggests using external guidance, in a form of predicates or terms, to guide interpolation. In contrast, GSpacer uses global guidance, based on the current proof, to direct different local generalization strategies. Thus, the guidance is automatically tuned to the specific instance at hand rather than to a domain of problems.

Global Invariant Inference. An alternative to inferring lemmas for the inductive invariant by blocking counterexamples is to enumerate the space of potential candidate invariants [9,14–16,28]. This does not suffer from the pitfall of local reasoning. However, it is only effective when the search space is constrained. While these approaches perform well on their target domain, they do not generalize well to a diverse set of benchmarks, as illustrated by results of CHC-COMP and our empirical evaluation in Sect. 5.

Locality in SMT and IMC. Local reasoning is also a known issue in SMT, and, in particular, in DPLL(T) (e.g., [22]). However, we are not aware of global guidance techniques for SMT solvers. Interpolation-based Model Checking (IMC) [20,21] that uses interpolants from proofs, inherits the problem. Compared to IMC, the propagation phase and inductive generalization of IC3 [7], can be seen as providing global guidance using lemmas found in other parts of the search-space. In contrast, GSpacer magnifies such global guidance by exploiting patterns within the lemmas themselves.

IC3-SMT-based Model Checkers. There are a number of IC3-style SMT-based infinite state model checkers, including [11,17,18]. To our knowledge, none extend the IC3-SMT framework with a global guidance. A rule similar to `Subsume` is suggested in [26] for the theory of bit-vectors and in [4] for LRA, but in both cases without global guidance. In [4], it is implemented via a combination of syntactic closure with interpolation, whereas we use MBP instead of interpolation. Refinement State Mining in [3] uses similar insights to our `Subsume` rule to refine predicate abstraction.

7 Conclusion and Future Work

This paper introduces *global guidance* to mitigate the limitations of the local reasoning performed by SMT-based IC3-style model checking algorithms. Global guidance is necessary to redirect such algorithms from divergence due to persistent local reasoning. To this end, we present three general rules that introduce new lemmas and POBs by taking a global view of the lemmas learned so far. The new rules are not theory-specific, and, as demonstrated by Algorithm 5, can

be incorporated to IC3-style solvers without modifying existing architecture. We instantiate, and implement, the rules for LIA in GSpacer, which extends Spacer.

Our evaluation shows that global guidance brings significant improvements to local reasoning, and surpasses invariant inference based solely on global reasoning. More importantly, global guidance decouples Spacer's dependency on interpolation strategy and performs almost equally well under all three interpolation schemes we consider. As such, using global guidance in the context of theories for which no good interpolation procedure exists, with bit-vectors being a primary example, arises as a promising direction for future research.

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Towards Model Checking Real-World Software-Defined Networks

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Abstract. In software-defined networks (SDN), a controller program is in charge of deploying diverse network functionality across a large number of switches, but this comes at a great risk: deploying buggy controller code could result in network and service disruption and security loopholes. The automatic detection of bugs or, even better, verification of their absence is thus most desirable, yet the size of the network and the complexity of the controller makes this a challenging undertaking. In this paper, we propose MOCS, a highly expressive, optimised SDN model that allows capturing subtle real-world bugs, in a reasonable amount of time. This is achieved by (1) analysing the model for possible partial order reductions, (2) statically pre-computing packet equivalence classes and (3) indexing packets and rules that exist in the model. We demonstrate its superiority compared to the state of the art in terms of expressivity, by providing examples of realistic bugs that a prototype implementation of MOCS in Uppaal caught, and performance/scalability, by running examples on various sizes of network topologies, highlighting the importance of our abstractions and optimisations.

1 Introduction

Software-Defined Networking (SDN) [16] has brought about a paradigm shift in designing and operating computer networks. A logically centralised controller implements the control logic and 'programs' the data plane, which is defined by flow tables installed in network switches. SDN enables the rapid development of advanced and diverse network functionality; e.g. in designing next-generation inter-data centre traffic engineering [10], load balancing [19], firewalls [24], and Internet exchange points (IXPs) [15]. SDN has gained noticeable ground in the industry, with major vendors integrating OpenFlow [37], the de-facto SDN standard maintained by the Open Networking Forum, in their products. Operators deploy it at scale [27,38]. SDN presents a unique opportunity for innovation and rapid development of complex network services by enabling all players, not just vendors, to develop and deploy control and data plane functionality in networks. This comes at a great risk; deploying buggy code at the controller could result in problematic flow entries at the data plane and, potentially, service disruption [13,18,47,49] and security loopholes [7,26]. Understanding and fixing such

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bugs is far from trivial, given the distributed and concurrent nature of computer networks and the complexity of the control plane [44].

With the advent of SDN, a large body of research on verifying network properties has emerged [33]. Static network analysis approaches [2,11,30,34,45,51] can only verify network properties on a given fixed network configuration but this may be changing very quickly (e.g. as in [1]). Another key limitation is the fact that they cannot reason about the controller program, which, itself, is responsible for the changes in the network configuration. Dynamic approaches, such as [23,29,31,40,48,50], are able to reason about network properties as changes happen (i.e. as flow entries in switches' flow tables are being added and deleted), but they cannot reason about the controller program either. As a result, when a property violation is detected, there is no straightforward way to fix the bug in the controller code, as these systems are oblivious of the running code. Identifying bugs in large and complex deployments can be extremely challenging.

Formal verification methods that include the controller code in the model of the network can solve this important problem. Symbolic execution methods, such as [5,8,11,12,14,28,46], evaluate programs using symbolic variables accumulating path-conditions along the way that then can be solved logically. However, they suffer from the path explosion problem caused by loops and function calls which means verification does not scale to larger controller programs (bug finding still works but is limited). Model checking SDNs is a promising area even though only few studies have been undertaken [3,8,28,35,36,43]. Networks and controller can be naturally modelled as transition systems. State explosion is always a problem but can be mitigated by using abstraction and optimisation techniques (i.e. partial order reductions). At the same time, modern model checkers [6,9,20,21,25] are very efficient.

NetSMC [28] uses a bespoke *symbolic* model checking algorithm for checking properties given a subset of computation tree logic that allows quantification only over all paths. As a result, this approach scales relatively well, but the requirement that only one packet can travel through the network at any time is very restrictive and ignores race conditions. NICE [8] employs model checking but only looks at a limited amount of input packets that are extracted through symbolically executing the controller code. As a result, it is a bug-finding tool only. The authors in [43] propose a model checking approach that can deal with dynamic controller updates and an arbitrary number of packets but require manually inserted non-interference lemmas that constrain the set of packets that can appear in the network. This significantly limits its applicability in realistic network deployments. Kuai [35] overcomes this limitation by introducing model-specific partial order reductions (PORs) that result in pruning the state space by avoiding redundant explorations. However, it has limitations explained at the end of this section.

In this paper, we take a step further towards the full realisation of model checking real-world SDNs by introducing MOCS (MOdel Checking for Software defined networks)[1], a highly expressive, optimised SDN model which we

[1] A release of MOCS is publicly available at https://tinyurl.com/y95qtv5k.

implemented in UPPAAL[2] [6]. MOCS, compared to the state of the art in model checking SDNs, can model network behaviour more realistically and verify larger deployments using fewer resources. The main contributions of this paper are:

Model Generality. The proposed network model is closer to the OpenFlow standard than previous models (e.g. [35]) to reflect commonly exhibited behaviour between the controller and network switches. More specifically, it allows for race conditions between control messages and includes a significant number of OpenFlow interactions, including barrier response messages. In our experimentation section, we present families of elusive bugs that can be efficiently captured by MOCS.

Model Checking Optimisations. To tackle the state explosion problem we propose context-dependent *partial order reductions* by considering the concrete control program and specification in question. We establish the soundness of the proposed optimisations. Moreover, we propose *state representation optimisations*, namely packet and rule indexing, identification of packet equivalence classes and bit packing, to improve performance. We evaluate the benefits from all proposed optimisations in Sect. 4.

Our model has been inspired by Kuai [35]. According to the contributions above, however, we consider MOCS to be a considerable improvement. We model more OpenFlow messages and interactions, enabling us to check for bugs that [35] cannot even express (see discussion in Sect. 4.2). Our context-dependent PORs systematically explore possibilities for optimisation. Our optimisation techniques still allow MOCS to run at least as efficiently as Kuai, often with even better performance.

2 Software-Defined Network Model

A key objective of our work is to enable the verification of network-wide properties in real-world SDNs. In order to fulfill this ambition, we present an extended network model to capture complex interactions between the SDN controller and the network. Below we describe the adopted network model, its state and transitions.

2.1 Formal Model Definition

The formal definition of the proposed SDN model is by means of an action-deterministic transition system. We parameterise the model by the underlying network topology λ and the controller program CP in use, as explained further below (Sect. 2.2).

Definition 1. *An SDN model is a 6-tuple* $\mathcal{M}_{(\lambda,\text{CP})} = (S, s_0, A, \hookrightarrow, AP, L)$*, where* S *is the set of all states the SDN may enter,* s_0 *the initial state,* A *the set of*

[2] UPPAAL has been chosen as future plans include extending the model to timed actions like e.g. timeouts. Note that the model can be implemented in any model checker.

actions which encode the events the network may engage in, $\hookrightarrow \subseteq S \times A \times S$ *the transition relation describing which execution steps the system undergoes as it perform actions, AP a set of atomic propositions describing relevant state properties, and* $L : S \to 2^{AP}$ *is a labelling function, which relates to any state* $s \in S$ *a set* $L(s) \in 2^{AP}$ *of those atomic propositions that are true for s. Such an SDN model is composed of several smaller systems, which model network components (hosts, switches and the controller) that communicate via queues and, combined, give rise to the definition of* $\hookrightarrow$*. The states of an SDN transition system are 3-tuples* (π, δ, γ)*, where* π *represents the state of each host,* δ *the state of each switch, and* γ *the controller state. The components are explained in Sect. 2.2 and the transitions* $\hookrightarrow$ *in Sect. 2.3.*

Figure 1 illustrates a high-level view of OpenFlow interactions (left side), modelled actions and queues (right side).

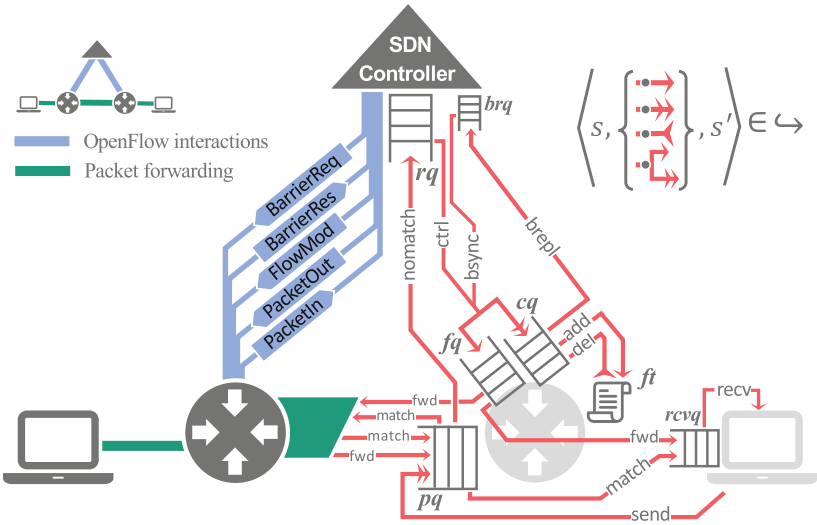


Fig. 1. A high-level view of OpenFlow interactions using OpenFlow specification terminology (left half) and the modelled actions (right half). A red solid-line arrow depicts an action which, when fired, (1) dequeues an item from the queue the arrow begins at, and (2) adds an item in the queue the arrowhead points to (or multiple items if the arrow is double-headed). Deleting an item from the target queue is denoted by a reverse arrowhead. A forked arrow denotes multiple targeted queues. (Color figure online)

2.2 SDN Model Components

Throughout we will use the common "dot-notation" (_._) to refer to components of composite gadgets (tuples), e.g. queues of switches, or parts of the state. We use obvious names for the projections functions like *s.δ.sw.pq* for the packet

queue of the switch sw in state s. At times we will also use t_1 and t_2 for the first and second projection of tuple t.

Network Topology. A location (n, pt) is a pair of a node (host or switch) n and a port pt. We describe the network topology as a bijective function $\lambda : (Switches \cup Hosts) \times Ports \rightarrow (Switches \cup Hosts) \times Ports$ consisting of a set of directed edges $\langle (n, pt), (n', pt') \rangle$, where pt' is the input port of the switch or host n' that is connected to port pt at host or switch n. *Hosts*, *Switches* and *Ports* are the (finite) sets of all hosts, switches and ports in the network, respectively. The topology function is used when a packet needs to be forwarded in the network. The location of the next hop node is decided when a *send*, *match* or *fwd* action (all defined further below) is fired. Every SDN model is w.r.t. a fixed topology λ that does not change.

Packets. Packets are modelled as finite bit vectors and transferred in the network by being stored to the queues of the various network components. A $packet \in Packets$ (the set of all packets that can appear in the network) contains bits describing the proof-relevant header information and its location *loc*.

Hosts. Each $host \in Hosts$, has a packet queue (*rcvq*) and a finite set of ports which are connected to ports of other switches. A host can send a packet to one or more switches it is connected to (*send* action in Fig. 1) or receive a packet from its own *rcvq* (*recv* action in Fig. 1). Sending occurs repeatedly in a non-deterministic fashion which we model implicitly via the $(0, \infty)$ abstraction at switches' packet queues, as discussed further below.

Switches. Each $switch \in Switches$, has a flow table (*ft*), a packet queue (*pq*), a control queue (*cq*), a forwarding queue (*fq*) and one or more ports, through which it is connected to other switches and/or hosts. A flow table $ft \subseteq Rules$ is a set of forwarding rules (with *Rules* being the set of all rules). Each one consists of a tuple $(priority, pattern, ports)$, where $priority \in \mathbb{N}$ determines the priority of the rule over others, *pattern* is a proposition over the proof-relevant header of a packet, and *ports* is a subset of the switch's ports. Switches match packets in their packet queues against rules (i.e. their respective *pattern*) in their flow table (*match* action in Fig. 1) and forward packets to a connected device (or final destination), accordingly. Packets that cannot be matched to any rule are sent to the controller's request queue (*rq*) (*nomatch* action in Fig. 1); in OpenFlow, this is done by sending a *PacketIn* message. The forwarding queue *fq* stores packets forwarded by the controller in *PacketOut* messages. The control queue stores messages sent by the controller in *FlowMod* and *BarrierReq* messages. *FlowMod* messages contain instructions to add or delete rules from the flow table (that trigger *add* and *del* actions in Fig. 1). *BarrierReq* messages contain barriers to synchronise the addition and removal of rules. MOCS conforms to the OpenFlow specifications and always execute instructions in an interleaved fashion obeying the ordering constraints imposed by barriers.

OpenFlow Controller. The controller is modelled as a finite state automaton embedded into the overall transition system. A controller program CP, as used to parametrise an SDN model, consists of $(CS, pktIn, barrierIn)$. It uses its own local state $cs \in CS$, where CS is the finite set of control program states. Incoming

PacketIn and *BarrierRes* messages from the SDN model are stored in separate queues (*rq* and *brq*, respectively) and trigger *ctrl* or *bsync* actions (see Fig. 1) which are then processed by the controller program in its current state. The controller's corresponding handler, *pktIn* for *PacketIn* messages and *barrierIn* for *BarrierRes* messages, responds by potentially changing its local state and sending messages to a subset of *Switches*, as follows. A number of *PacketOut* messages (pairs of *pkt*, *ports*) can be sent to a subset of *Switches*. Such a message is stored in a switch's forward queue and instructs it to forward packet *pkt* along the ports *ports*. The controller may also send any number of *FlowMod* and *BarrierReq* messages to the control queue of any subset of *Switches*. A *FlowMod* message may contain an *add* or *delete* rule modification instruction. These are executed in an arbitrary order by switches, and *barriers* are used to synchronise their execution. Barriers are sent by the controller in *BarrierReq* messages. OpenFlow requires that a response message (*BarrierRes*) is sent to the controller by a switch when a barrier is consumed from its control queue so that the controller can synchronise subsequent actions. Our model includes a *brepl* action that models the sending of a *BarrierRes* message from a switch to the controller's barrier reply queue (*brq*), and a *bsync* action that enables the controller program to react to barrier responses.

Queues. All queues in the network are modelled as *finite* state. Packet queues *pq* for switches are modelled as multisets, and we adopt $(0, \infty)$ abstraction [41]; i.e. a packet is assumed to appear either zero or an arbitrary (unbounded) amount of times in the respective multiset. This means that once a packet has arrived at a switch or host, (infinitely) many other packets of the same kind repeatedly arrive at this switch or host. Switches' forwarding queues *fq* are, by contrast, modelled as sets, therefore if multiple identical packets are sent by the controller to a switch, only one will be stored in the queue and eventually forwarded by the switch. The controller's request *rq* and barrier reply queues *brq* are modelled as sets as well. Hosts' receive queues *rcvq* are also modelled as sets. Controller queues *cq* at switches are modelled as a finite sequence of sets of control messages (representing add and remove rule instructions), interleaved by any number of barriers. As the number of barriers that can appear at any execution is finite, this sequence is finite.

2.3 Guarded Transitions

Here we provide a detailed breakdown of the transition relation $s \xrightarrow{\alpha(\vec{a})} s'$ for each action $\alpha(\vec{a}) \in A(s)$, where $A(s)$ the set of all enabled actions in s in the proposed model (see Fig. 1). Transitions are labelled by action names α with arguments $\vec{a}$. The transitions are only enabled in state s if s satisfies certain conditions called *guards* that can refer to the arguments $\vec{a}$. In guards, we make use of predicate $bestmatch(sw, r, pkt)$ that expresses that r is the highest priority rule in $sw.ft$ that matches pkt's header. Below we list all possible actions with their respective guards.

***send*(h, pt, pkt).** Guard: *true*. This transition models packets arriving in the network in a non-deterministic fashion. When it is executed, *pkt* is added to

the packet queue of the network switch connected to the port pt of host h (or, formally, to $\lambda(h, pt)_1.pq$, where λ is the topology function described above). As described in Sect. 3.2, only relevant representatives of packets are actually sent by end-hosts. This transition is unguarded, therefore it is always enabled.

***recv*(h, pkt).** Guard: $pkt \in h.rcvq$. This transition models hosts receiving (and removing) packets from the network and is enabled if pkt is in h's receive queue.

***match*(sw, pkt, r).** Guard: $pkt \in sw.pq \wedge r \in sw.ft \wedge bestmatch(sw, r, pkt)$. This transition models matching and forwarding packet pkt to zero or more next hop nodes (hosts and switches), as a result of highest priority matching of rule r with pkt. The packet is then copied to the packet queues of the connected hosts and/or switches, by applying the topology function to the port numbers in the matched rule; i.e. $\lambda(sw, pt)_1.pq, \forall pt \in r.ports$. Dropping packets is modelled by having a special 'drop' port that can be included in rules. The location of the forwarded packet(s) is updated with the respective destination (switch/host, port) pair; i.e. $\lambda(sw, pt)$. Due to the $(0, \infty)$ abstraction, the packet is not removed from $sw.pq$.

***nomatch*(sw, pkt).** Guard: $pkt \in sw.pq \wedge \nexists r \in sw.ft \ . \ bestmatch(sw, r, pkt)$. This transition models forwarding a packet to the OpenFlow controller when a switch does not have a rule in its forwarding table that can be matched against the packet header. In this case, pkt is added to rq for processing. pkt is not removed from $sw.pq$ due to the supported $(0, \infty)$ abstraction.

***ctrl*(sw, pkt, cs).** Guard: $pkt \in controller.rq$. This transition models the execution of the packet handler by the controller when packet pkt that was previously sent by sw is available in rq. The controller's packet handler function $pktIn(sw, pkt, cs)$ is executed which, in turn (i) reads the current controller state cs and changes it according to the controller program, (ii) adds a number of rules, interleaved with any number of barriers, into the cq of zero or more switches, and (iii) adds zero or more forwarding messages, each one including a packet along with a set of ports, to the fq of zero or more switches.

***fwd*$(sw, pkt, ports)$.** Guard: $(pkt, ports) \in sw.fq$. This transition models forwarding packet pkt that was previously sent by the controller to sw's forwarding queue $sw.fq$. In this case, pkt is removed from $sw.fq$ (which is modelled as a set), and added to the pq of a number of network nodes (switches and/or hosts), as defined by the topology function $\lambda(sw, pt)_1.pq, \forall pt \in ports$. The location of the forwarded packet(s) is updated with the respective destination (switch/host, port) pair; i.e. $\lambda(n, pt)$.

***FM*(sw, r)**, where $FM \in \{add, del\}$. Guard: $(FM, r) \in head(sw.cq)$. These transitions model the addition and deletion, respectively, of a rule in the flow table of switch sw. They are enabled when one or more add and del control messages are in the set at the head of the switch's control queue. In this case, r is added to – or deleted from, respectively – $sw.ft$ and the control message is deleted from the set at the head of cq. If the set at the head of cq becomes empty it is removed. If then the next item in cq is a barrier, a *brepl* transition becomes enabled (see below).

***brepl*(*sw*, *xid*).** Guard: $b(xid) = head(sw.cq)$. This transition models a switch sending a barrier response message, upon consuming a barrier from the head of its control queue; i.e. if $b(xid)$ is the head of $sw.cq$, where $xid \in \mathbb{N}$ is an identifier for the barrier set by the controller, $b(xid)$ is removed and the barrier reply message $br(sw, xid)$ is added to the controller's *brq*.

***bsync*(*sw*, *xid*, *cs*).** Guard: $br(sw, xid) \in controller.brq$. This transition models the execution of the barrier response handler by the controller when a barrier response sent by switch *sw* is available in *brq*. In this case, $br(sw, xid)$ is removed from the *brq*, and the controller's barrier handler $barrierIn(sw, xid, cs)$ is executed which, in turn (i) reads the current controller state *cs* and changes it according to the controller program, (ii) adds a number of rules, interleaved with any number of barriers, into the *cq* of zero or more switches, and (iii) adds zero or more forwarding messages, each one including a packet along with a set of ports, to the *fq* of zero or more switches.

An Example Run. In Fig. 2, we illustrate a sequence of MOCS transitions through a simple packet forwarding example. The run starts with a *send* transition; packet p is copied to the packet queue of the switch in black. Initially, switches' flow tables are empty, therefore p is copied to the controller's request queue (*nomatch* transition); note that p remains in the packet queue of the switch in black due to the $(0, \infty)$ abstraction. The controller's packet handler is then called (*ctrl* transition) and, as a result, (1) p is copied to the forwarding queue of the switch in black, (2) rule r_1 is copied to the control queue of the switch in black, and (3) rule r_2 is copied to the control queue of the switch in white. Then, the switch in black forwards p to the packet queue of the switch in white (*fwd* transition). The switch in white installs r_2 in its flow table (*add* transition) and then matches p with the newly installed rule and forwards it to the receive queue of the host in white (*match* transition), which removes it from the network (*recv* transition).

2.4 Specification Language

In order to specify properties of packet flow in the network, we use LTL formulas without "next-step" operator $\bigcirc$[3], where atomic formulae denoting properties of states of the transition system, i.e. SDN network. In the case of safety properties, i.e. an invariant w.r.t. states, the $\text{LTL}_{\setminus\{\bigcirc\}}$ formula is of the form $\Box\varphi$, i.e. has only an outermost $\Box$ temporal connective.

Let P denote unary predicates on packets which encode a property of a packet based on its fields. An atomic *state condition* (proposition) in AP is either of the following: (i) existence of a packet *pkt* located in a packet queue (*pq*) of a switch or in a receive queue (*rcvq*) of a host that satisfies P (we denote this by $\exists pkt{\in}n.pq\,.\,P(pkt)$ with $n \in Switches$, and $\exists pkt{\in}h.rcvq\,.\,P(pkt)$

[3] This is the largest set of formulae supporting the partial order reductions used in Sect. 3, as stutter equivalence does not preserve the truth value of formulae with the $\bigcirc$.

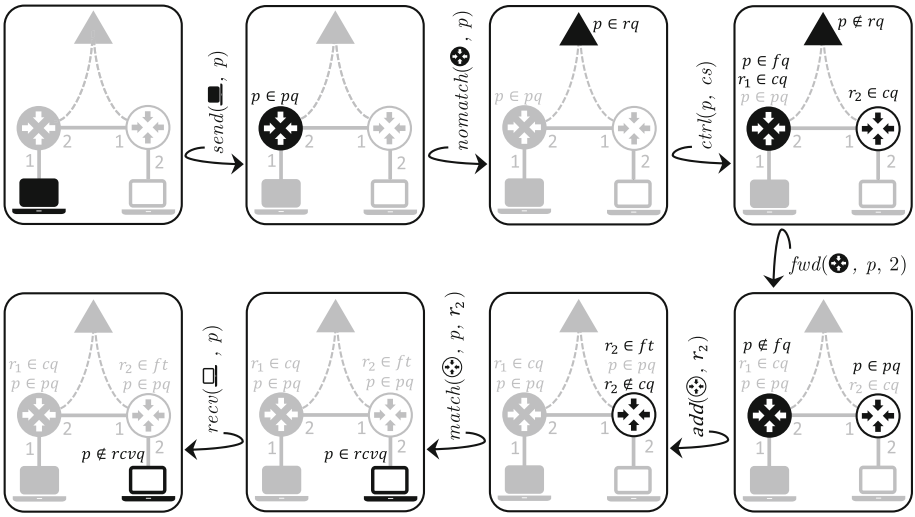


Fig. 2. Forwarding p from ■ to □. Non greyed-out icons are the ones whose state changes in the current transition.

with $h \in Hosts$)[4]; (ii) the controller is in a specific *controller* state $q \in CS$, denoted by a unary predicate symbol $Q(q)$ which holds in system state $s \in S$ if $q = s.\gamma.cs$. The specification logic comprises first-order formula with equality on the finite domains of switches, hosts, rule priorities, and ports which are *state-independent* (and decidable).

For example, $\exists pkt{\in}sw.pq\,.\,P(pkt)$ represents the fact that the packet predicate $P(\_)$ is true for at least one packet pkt in the pq of switch sw. For every atomic packet proposition $P(pkt)$, also its negation $\neg P(pkt)$ is an atomic proposition for the reason of simplifying syntactic checks of formulae in Table 1 in the next section. Note that universal quantification over packets in a queue is a derived notion. For instance, $\forall pkt{\in}n.pq\,.\,P(pkt)$ can be expressed as $\nexists pk{\in}n.pq\,.\,\neg P(pkt)$. Universal and existential quantification over switches or hosts can be expressed by finite iterations of $\wedge$ and $\vee$, respectively.

In order to be able to express that a condition holds when a certain event happened, we add to our propositions instances of *propositional dynamic logic* [17,42]. Given an action $\alpha(\cdot) \in A$ and a proposition P that may refer to any variables in $\vec{x}$, $[\alpha(\vec{x})]P$ is also a proposition and $[\alpha(\vec{x})]P$ is true if, and only if, after firing transition $\alpha(\vec{a})$ (to get to the current state), P holds with the variables in $\vec{x}$ bound to the corresponding values in the actual arguments $\vec{a}$. With the help of those basic modalities one can then also specify that more complex events occurred. For instance, dropping of a packet due to a *match* or *fwd* action can be expressed by $[match(sw, pkt, r)](r.fwd\_port = \texttt{drop}) \wedge [fwd(sw, pkt, pt)](pt = \texttt{drop})$. Such predicates derived from modalities are used in [32] (extended version of this paper, with proofs and controller programs), Appendix B-CP5.

[4] Note that these are *atomic* propositions despite the use of the existential quantifier notation.

The meaning of temporal LTL operators is standard depending on the trace of a transition sequence $s_0 \overset{\alpha_1}{\hookrightarrow} s_1 \overset{\alpha_2}{\hookrightarrow} \ldots$. The trace $L(s_0)L(s_1)\ldots L(s_i)\ldots$ is defined as usual. For instance, trace $L(s_0)L(s_1)L(s_2)\ldots$ satisfies invariant $\Box\varphi$ if each $L(s_i)$ implies φ.

3 Model Checking

In order to verify desired properties of an SDN, we use its model as described in Definition 1 and apply model checking. In the following we propose optimisations that significantly improve the performance of model checking.

3.1 Contextual Partial-Order Reduction

Partial order reduction (POR) [39] reduces the number of interleavings (traces) one has to check. Here is a reminder of the main result (see [4]) where we use a stronger condition than the regular (*C4*) to deal with cycles:

Theorem 1 (Correctness of POR). *Given a finite transition system $\mathcal{M} = (S, A, \hookrightarrow, s_0, AP, L)$ that is action-deterministic and without terminal states, let $A(s)$ denote the set of actions in A enabled in state $s \in S$. Let $ample(s) \subseteq A(s)$ be a set of actions for a state $s \in S$ that satisfies the following conditions:*

C1 (Non)emptiness condition: $\varnothing \neq ample(s) \subseteq A(s)$.

C2 Dependency condition: Let $s \overset{\alpha_1}{\hookrightarrow} s_1 \ldots \overset{\alpha_n}{\hookrightarrow} s_n \overset{\beta}{\hookrightarrow} t$ be a run in $\mathcal{M}$. If $\beta \in A \setminus ample(s)$ depends on $ample(s)$, then $\alpha_i \in ample(s)$ for some $0 < i \leqslant n$, which means that in every path fragment of $\mathcal{M}$, β cannot appear before some transition from $ample(s)$ is executed.

C3 Invisibility condition: If $ample(s) \neq A(s)$ (i.e., state s is not fully expanded), then every $\alpha \in ample(s)$ is invisible.

C4 Every cycle in $\mathcal{M}^{ample}$ contains a state s such that $ample(s) = A(s)$.

where $\mathcal{M}^{ample} = (S_a, A, \hookrightarrow\!\!\!\!\rightarrow, s_0, AP, L_a)$ is the new, optimised, model defined as follows: let $S_a \subseteq S$ be the set of states reachable from the initial state s_0 under $\hookrightarrow\!\!\!\!\rightarrow$, let $L_a(s) = L(s)$ for all $s \in S_a$, and define $\hookrightarrow\!\!\!\!\rightarrow \subseteq S_a \times A \times S_a$ inductively by the rule

$$\frac{s \overset{\alpha}{\hookrightarrow} s'}{s \overset{\alpha}{\hookrightarrow\!\!\!\!\rightarrow} s'} \qquad \text{if} \quad \alpha \in ample(s)$$

If $ample(s)$ satisfies conditions (C1)–(C4) as outlined above, then for each path in $\mathcal{M}$ there exists a stutter-trace equivalent path in $\mathcal{M}^{ample}$, and vice-versa, denoted $\mathcal{M} \overset{\text{st}}{\equiv} \mathcal{M}^{ample}$.

The intuitive reason for this theorem to hold is the following: Assume an action sequence $\alpha_i \ldots \alpha_{i+n}\beta$ that reaches the state s, and β is *independent* of $\{\alpha_i, \ldots \alpha_{i+n}\}$. Then, one can permute β with α_{i+n} through α_i successively n times. One can

therefore construct the sequence $\beta\alpha_i ... \alpha_{i+n}$ that also reaches the state s. If this shift of β does not affect the labelling of the states with atomic propositions (β is called *invisible* in this case), then it is not detectable by the property to be shown and the permuted and the original sequence are equivalent w.r.t. the property and thus don't have to be checked both. One must, however, ensure, that in case of loops (infinite execution traces) the ample sets do not *preclude* some actions to be fired altogether, which is why one needs (*C4*).

The more actions that are both stutter and provably independent (also referred to as *safe actions* [22]) there are, the smaller the transition system, and the more efficient the model checking. One of our contributions is that we attempt to identify *as many safe actions as possible* to make PORs more widely applicable to our model.

The PORs in [35] consider only dependency and invisibility of *recv* and *barrier* actions, whereas we explore systematically all possibilities for applications of Theorem 1 to reduce the search space. When identifying safe actions, we consider (1) the actual controller program CP, (2) the topology λ and (3) the state formula φ to be shown invariant, which we call the *context* CTX of actions. It turns out that two actions may be dependent in a given context of abstraction while independent in another context, and similarly for invisibility, and we exploit this fact. The argument of the action thus becomes relevant as well.

Definition 2 (Safe Actions). *Given a context* $\text{CTX} = (\text{CP}, \lambda, \varphi)$*, and SDN model* $\mathcal{M}_{(\lambda,\text{CP})} = (S, A, \hookrightarrow, s_0, AP, L)$*, an action* $\alpha(\cdot) \in A(s)$ *is called 'safe' if it is independent of any other action in* A *and invisible for* φ*. We write safe actions* $\check{\alpha}(\cdot)$*.*

Definition 3 (Order-sensitive Controller Program). *A controller program* CP *is order-sensitive if there exists a state* $s \in S$ *and two actions* α, β *in* $\{ctrl(\cdot), bsync(\cdot)\}$ *such that* $\alpha, \beta \in A(s)$ *and* $s \overset{\alpha}{\hookrightarrow} s_1 \overset{\beta}{\hookrightarrow} s_2$ *and* $s \overset{\beta}{\hookrightarrow} s_3 \overset{\alpha}{\hookrightarrow} s_4$ *with* $s_2 \neq s_4$*.*

Definition 4. *Let* φ *be a state formula. An action* $\alpha \in A$ *is called '*φ*-invariant' if* $s \models \varphi$ *iff* $\alpha(s) \models \varphi$ *for all* $s \in S$ *with* $\alpha \in A(s)$*.*

Lemma 1. *For transition system* $\mathcal{M}_{(\lambda,\text{CP})} = (S, A, \hookrightarrow, s_0, AP, L)$ *and a formula* $\varphi \in LTL_{\setminus\{\bigcirc\}}$*,* $\alpha \in A$ *is safe* iff $\bigwedge_{i=1}^{3} Safe_i(\alpha)$*, where* $Safe_i$*, given in Table 1, are per-row.*

Proof. See [32] Appendix A.

Theorem 2 (POR instance for SDN). *Let* $(\text{CP}, \lambda, \varphi)$ *be a context such that* $\mathcal{M}_{(\lambda,\text{CP})} = (S, A, \hookrightarrow, s_0, AP, L)$ *is an SDN network model from Definition 1; and let safe actions be as in Definition 2. Further, let* $ample(s)$ *be defined by:*

$$ample(s) = \begin{cases} \{\alpha \in A(s) \mid \alpha \text{ safe } \} & \text{if } \{\alpha \in A(s) \mid \alpha \text{ safe } \} \neq \varnothing \\ A(s) & \text{otherwise} \end{cases}$$

Table 1. Safeness predicates

Action $Safe_1(\alpha)$	Independence $Safe_2(\alpha)$	Invisibility $Safe_3(\alpha)$
$\alpha = ctrl(sw, pk, cs)$	CP is not order-sensitive	**if** $Q(q)$ occurs in φ, where $q \in CS$, **then** α is φ-invariant
$\alpha = bsync(sw, xid, cs)$	CP is not order-sensitive	**if** $Q(q)$ occurs in φ, where $q \in CS$, **then** α is φ-invariant
$\alpha = fwd(sw, pk, ports)$	$\top$	**if** $\exists pk \in b.q \,.\, P(pk)$ occurs in φ, for any $b \in \{sw\} \cup \{\lambda(sw, p)_1 \mid p \in ports\}$ and $q \in \{pq, recvq\}$, **then** α is φ-invariant
$\alpha = brepl(sw, xid)$	$\top$	$\top$
$\alpha = recv(h, pk)$	$\top$	**if** $\exists pk \in h.rcvq \,.\, P(pk)$ occurs in φ, **then** α is φ-invariant

Then, ample satisfies the criteria of Theorem 1 and thus $\mathcal{M}_{(\lambda,\text{CP})} \overset{\text{st}}{\equiv} \mathcal{M}^{ample}_{(\lambda,\text{CP})}$ [5]

Proof.

C1 The (non)emptiness condition is trivial since by definition of $ample(s)$ it follows that $ample(s) = \varnothing$ iff $A(s) = \varnothing$.

C2 By assumption $\beta \in A \backslash ample(s)$ depends on $ample(s)$. But with our definition of $ample(s)$ this is impossible as all actions in $ample(s)$ are safe and by definition independent of all other actions.

C3 The validity of the invisibility condition is by definition of *ample* and safe actions.

C4 We now show that every cycle in $\mathcal{M}^{ample}_{(\lambda,\text{CP})}$ contains a fully expanded state s, i.e. a state s such that $ample(s) = A(s)$. By definition of $ample(s)$ in Theorem 2 it is equivalent to show that there is no cycle in $\mathcal{M}^{ample}_{(\lambda,\text{CP})}$ consisting of safe actions only. We show this by contradiction, assuming such a cycle of only safe actions exists. There are five safe action types to consider: *ctrl*, *fwd*, *brepl*, *bsync* and *recv*. Distinguish two cases.

Case 1. A sequence of safe actions of same type. Let us consider the different safe actions:

- Let ρ an execution of $\mathcal{M}^{ample}_{(\lambda,\text{CP})}$ which consists of only one type of *ctrl*-actions:

$$\rho = s_1 \xrightarrow{ctrl(pkt_1, cs_1)} s_2 \xrightarrow{ctrl(pkt_2, cs_2)} \ldots s_{i-1} \xrightarrow{ctrl(pkt_{i-1}, cs_{i-1})} s_i$$

  Suppose ρ is a cycle. According to the *ctrl* semantics, for each transition $s \xrightarrow{ctrl(pkt, cs)} s'$, where $s = (\pi, \delta, \gamma)$, $s' = (\pi', \delta', \gamma')$, it holds that $\gamma'.rq = \gamma.rq \backslash \{pkt\}$ as we use sets to represent rq buffers. Hence, for the execution ρ it holds $\gamma_i.rq = \gamma_1.rq \backslash \{pkt_1, pkt_2, \ldots pkt_{i-1}\}$ which implies that $s_1 \neq s_i$. Contradiction.

[5] Stutter equivalence here implicitly is defined w.r.t. the atomic propositions appearing in φ, but this suffices as we are just interested in the validity of φ.

- Let ρ an execution which consists of only one type of *fwd*-actions: similar argument as above since *fq*-s are represented by sets and thus forward messages are removed from *fq*.
- Let ρ an execution which consists of only one type of *brepl*-actions: similar argument as above since control messages are removed from *cq*.
- Let ρ an execution which consists of only one type of *bsync*-actions: similar argument as above, as barrier reply messages are removed from *brq*-s that are represented by sets.
- Let ρ an execution which consists of only one type of *recv*-actions: similar argument as above, as packets are removed from *rcvq* buffers that are represented by sets.

Case 2. A sequence of different safe actions. Suppose there exists a cycle with mixed safe actions starting in s_1 and ending in s_i. Distinguish the following cases.

i) There exists at least a *ctrl* and/or a *bsync* action in the cycle. According to the effects of safe transitions, the *ctrl* action will change to a state with smaller *rq* and the *bsync* will always switch to a state with smaller *brq*. It is important here that *ctrl* does not interfere with *bsync* regarding *rq, brq*, and no safe action of other type than *ctrl* and *bsync* accesses *rq* or *brq*. This implies that $s_1 \neq s_i$. Contradiction.
ii) Neither *ctrl*, nor *bsync* actions in the cycle.
   a) There is a *fwd* and/or *brepl* in the cycle: *fwd* will always switch to a state with smaller *fq* and *brepl* will always switch to a state with smaller *cq* (*brepl* and *recv* do not interfere with *fwd*). This implies that $s_1 \neq s_i$. Contradiction.
   b) There is neither *fwd* nor *brepl* in the cycle. This means that only *recv* is in the cycle which is already covered by the first case.

□

Due to the definition of the transition system via ample sets, each safe action is immediately executed after its enabling one. Therefore, one can merge every transition of a safe action with its precursory enabling one. Intuitively, the semantics of the merged action is defined as the successive execution of its constituent actions. This process can be repeated if there is a chain of safe actions; for instance, in the case of $s \xhookrightarrow{nomatch(sw,pkt)} s' \xhookrightarrow{ctrl(sw,pkt,cs)} s'' \xhookrightarrow{fwd(sw,pkt,ports)} s'''$ where each transition enables the next and the last two are assumed to be safe. These transitions can be merged into one, yielding a stutter equivalent trace as the intermediate states are invisible (w.r.t. the context and thus the property to be shown) by definition of safe actions.

3.2 State Representation

Efficient state representation is crucial for minimising MOCS's memory footprint and enabling it to scale up to relatively large network setups.

Packet and Rule Indexing. In MOCS, only a single instance of each packet and rule that can appear in the modelled network is kept in memory. An index is then used to associate queues and flow tables with packets and rules, with a single bit indicating their presence (or absence). This data structure is illustrated in Fig. 3. For a data packet, a value of 1 in the *pq* section of the entry indicates that infinite copies of it are stored in the packet queue of the respective switch. A value of 1 in the *fq* section indicates that a single copy of the packet is stored in the forward queue of the respective switch. A value of 1 in the *rq* section indicates that a copy of the packet sent by the respective switch (when a *nomatch* transition is fired) is stored in the controller's request queue. For a rule, a value of 1 in the *ft* section indicates that the rule is installed in the respective switch's flow table. A value of 1 in the *cq* section indicates that the rule is part of a *FlowMod* message in the respective switch's control queue.

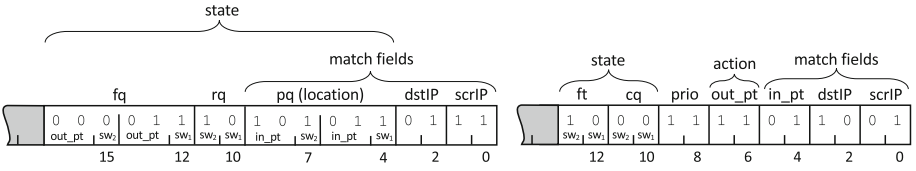


Fig. 3. Packet (left) and rule (right) indices

The proposed optimisation enables scaling up the network topology by minimising the required memory footprint. For every switch, MOCS only requires a few bits in each packet and rule entry in the index.

Discovering Equivalence Classes of Packets. Model checking with all possible packets, including all specified fields in the OpenFlow standard, would entail a huge state space that would render any approach unusable. Here, we propose the discovery of equivalence classes of packets that are then used for model checking. We first remove all fields that are not referenced in a statement or rule creation or deletion in the controller program. Then, we identify packet classes that would result in the same controller behaviour. Currently, as with the rest of literature, we focus on simple controller programs where such equivalence classes can be easily identified by analysing static constraints and rule manipulation in the controller program. We then generate one representative packet from each class and assign it to all network switches that are directly connected to end-hosts; i.e. modelling clients that can send an arbitrarily large number of packets in a non-deterministic fashion. We use the minimum possible number of bits to represent the identified equivalence classes. For example, if the controller program exerts different behaviour if the destination TCP port of a packet is 23 (i.e. destined to an SSH server) or not, we only use a 1-bit field to model this behaviour.

Bit Packing. We reduce the size of each recorded state by employing bit packing using the *int* type supported by UPPAAL, and bit-level operations for the entries in the packet and rule indices as well as for the packets and rules themselves.

4 Experimental Evaluation

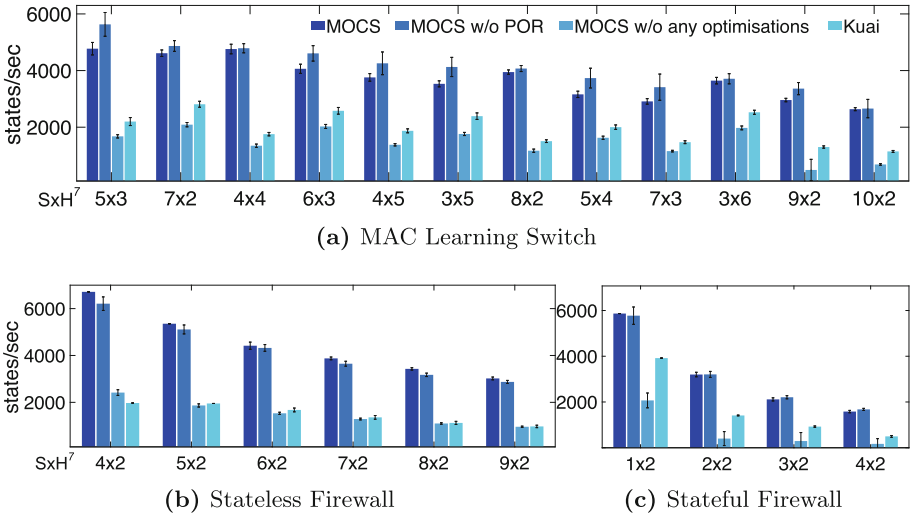
In this section, we experimentally evaluate MOCS by comparing it with the state of the art, in terms of performance (verification throughput and memory footprint) and model expressivity. We have implemented MOCS in UPPAAL [6] as a network of parallel automata for the controller and network switches, which communicate asynchronously by writing/reading packets to/from queues that are part of the model discussed in Sect. 2. As discussed in Sect. 3, this is implemented by directly manipulating the packet and rule indices.

Throughout this section we will be using three examples of network controllers: (1) A *stateless firewall* ([32] Appendix B-CP1) requires the controller to install rules to network switches that enable them to decide whether to forward a packet towards its destination or not; this is done in a stateless fashion, i.e. without having to consider any previously seen packets. For example, a controller could configure switches to block all packets whose destination TCP port is 22 (i.e. destined to an SSH server). (2) A *stateful firewall* ([32] Appendix B-CP2) is similar to the stateless one but decisions can take into account previously seen packets. A classic example of this is to allow bi-directional communication between two end-hosts, when one host opens a TCP connection to the other. Then, traffic flowing from the other host back to the connection initiator should be allowed to go through the switches on the reverse path. (3) A *MAC learning application* ([32] Appendix B-CP3) enables the controller and switches to learn how to forward packets to their destinations (identified with respective MAC addresses). A switch sends a *PacketIn* message to the controller when it receives a packet that it does not know how to forward. By looking at this packet, the controller learns a mapping of a source switch (or host) to a port of the requesting switch. It then installs a rule (by sending a *FlowMod* message) that will allow that switch to forward packets back to the source switch (or host), and asks the requesting switch (by sending a *PacketOut* message) to flood the packet to all its ports except the one it received the packet from. This way, the controller eventually learns all mappings, and network switches receive rules that enable them to forward traffic to their neighbours for all destinations in the network.

4.1 Performance Comparison

We measure MOCS's performance, and also compare it against Kuai [35][6] using the examples described above, and we investigate the behaviour of MOCS as we scale up the network (switches and clients/servers). We report three metrics:

[6] Note that parts of Kuai's source code are not publicly available, therefore we implemented it's model in UPPAAL.



(a) MAC Learning Switch

(b) Stateless Firewall

(c) Stateful Firewall

Fig. 4. Performance comparison – verification throughput

(1) *verification throughput* in visited states per second, (2) number of visited states, and (3) required memory. We have run all verification experiments on an 18-Core iMac pro, 2.3 GHz Intel Xeon W with 128 GB DDR4 memory.

Verification Throughput. We measure the verification throughput when running a single experiment at a time on one CPU core and report the average and standard deviation for the first 30 min of each run. In order to assess how MOCS's different optimisations affect its performance, we report results for the following system variants: (1) MOCS, (2) MOCS without POR, (3) MOCS without any optimisations (neither POR, state representation), and (4) Kuai. Figure 4 shows the measured throughput (with error bars denoting standard deviation).

For the MAC learning and stateless firewall applications, we observe that MOCS performs significantly better than Kuai for all different network setups and sizes[7], achieving at least double the throughput Kuai does. The throughput performance is much better for the stateful firewall, too. This is despite the fact that, for this application, Kuai employs the unrealistic optimisation where the *barrier* transition forces the immediate update of the forwarding state. In other words, MOCS is able to explore significantly more states and identify bugs that Kuai cannot (see Sect. 4.2).

The computational overhead induced by our proposed PORs is minimal. This overhead occurs when PORs require dynamic checks through the safety predicates described in Table 1. This is shown in Fig. 4a, where, in order to decide about the (in)visibility of *fwd(sw,pk,pt)* actions, a lookup is performed in the history-array of packet *pk*, checking whether the bit which corresponds to switch sw', which is connected with port *pt* of *sw*, is set. On the other hand, if a POR does not require any dynamic checks, no penalty is induced, as shown in Figs. 4b

[7] S × H in Figs. 4 to 6 indicates the number of switches S and hosts H.

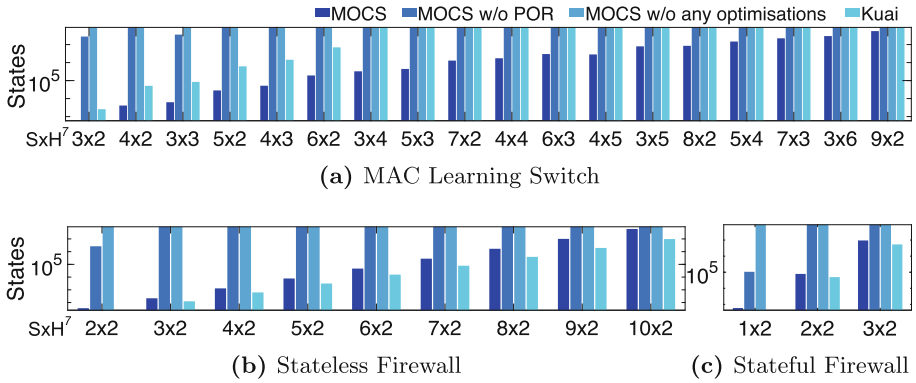


Fig. 5. Performance comparison – visited states (logarithmic scale)

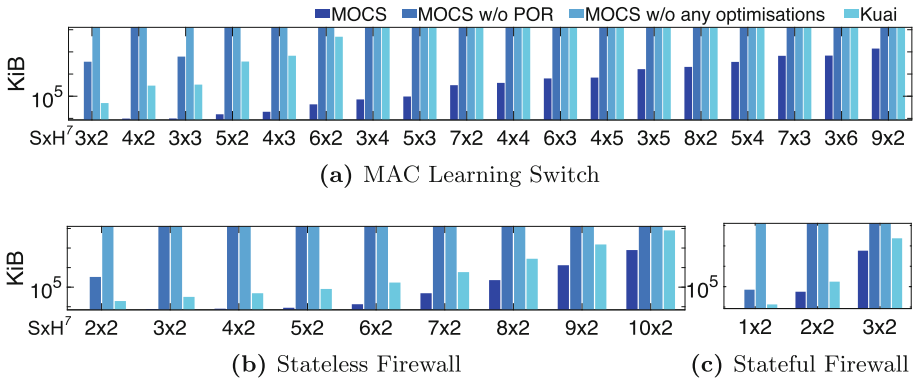


Fig. 6. Performance comparison – memory footprint (logarithmic scale)

and 4c, where the throughput when the PORs are disabled is almost identical to the case where PORs are enabled. This is because it has been statically established at a pre-analysis stage that all actions of a particular type are always safe for any argument/state. It is important to note that even when computational overhead is induced, PORs enable MOCS to scale up to larger networks because the number of visited states can be significantly reduced, as discussed below.

In order to assess the contribution of the state representation optimisation in MOCS's performance, we measure the throughput when both PORs and state representation optimisations are disabled. It is clear that they contribute significantly to the overall throughput; without these the measured throughput was at least less than half the throughput when they were enabled.

Number of Visited States and Required Memory. Minimising the number of visited states and required memory is crucial for scaling up verification to larger networks. The proposed partial order reductions (Sect. 3.1) and identification of packet equivalent classes aim at the former, while packet/rule indexing

and bit packing aim at the latter (§3.2). In Fig. 5, we present the results for the various setups and network deployments discussed above. We stopped scaling up the network deployment for each setup when the verification process required more than 24 h or started swapping memory to disk. For these cases we killed the process and report a topped-up bar in Figs. 5 and 6.

For the MAC learning application, MOCS can scale up to larger network deployments compared to Kuai, which could not verify networks consisting of more than 2 hosts and 6 switches. For that network deployment, Kuai visited ∼7 m states, whereas MOCS visited only ∼193 k states. At the same time, Kuai required around 48 GBs of memory (7061 bytes/state) whereas MOCS needed ∼43 MBs (228 bytes/state). Without the partial order reductions, MOCS can only verify tiny networks. The contribution of the proposed state representation optimisations is also crucial; in our experiments (results not shown due to lack of space), for the 6×2 network setups (the largest we could do without these optimisations), we observed a reduction in state space (due to the identification of packet equivalence classes) and memory footprint (due to packet/rule indexing and bit packing) from ∼7 m to ∼200k states and from ∼6 KB per state to ∼230 B per state. For the stateless and stateful firewall applications, resp., MOCS performs equally well to Kuai with respect to scaling up.

4.2 Model Expressivity

The proposed model is significantly more expressive compared to Kuai as it allows for more asynchronous concurrency. To begin with, in MOCS, controller messages sent before a barrier request message can be interleaved with all other enabled actions, other than the control messages sent after the barrier. By contrast, Kuai always flushes all control messages until the last barrier in one go, masking a large number of interleavings and, potentially, buggy behaviour. Next, in MOCS *nomatch, ctrl* and *fwd* can be interleaved with other actions. In Kuai, it is enforced a mutual exclusion concurrency control policy through the *wait*-semaphore: whenever a *nomatch* occurs the mutex is locked and it is unlocked by the *fwd* action of the thread *nomatch-ctrl-fwd* which refers to the same packet; all other threads are forced to wait. Moreover, MOCS does not impose any limit on the size of the *rq* queue, in contrast to Kuai where only one packet can exist in it. In addition, Kuai does not support notifications from the data plane to the controller for completed operations as it does not support reply messages and as a result any bug related to the fact that the controller is not synced to data-plane state changes is hidden.[8] Also, our specification language for states is more expressive than Kuai's, as we can use any property in LTL without "next", whereas Kuai only uses invariants with a single outermost $\Box$.

The MOCS extensions, however, are conservative with respect to Kuai, that is we have the following theorem (without proof, which is straightforward):

[8] There are further small extensions; for instance, in MOCS the controller can send multiple *PacketOut* messages (as OpenFlow prescribes).

Theorem 3 (MOCS Conservativity). *Let* $\mathcal{M}_{(\lambda,\text{CP})} = (S, A, \hookrightarrow, s_0, AP, L)$ *and* $\mathcal{M}^{K}_{(\lambda,\text{CP})} = (S_K, A_K, \hookrightarrow_K, s_0, AP, L)$ *the original SDN models of MOCS and Kuai, respectively, using the same topology and controller. Furthermore, let* $Traces(\mathcal{M}_{(\lambda,\text{CP})})$ *and* $Traces(\mathcal{M}^{K}_{(\lambda,\text{CP})})$ *denote the set of all initial traces in these models, respectively. Then,* $Traces(\mathcal{M}^{K}_{(\lambda,\text{CP})}) \subseteq Traces(\mathcal{M}_{(\lambda,\text{CP})})$.

For each of the extensions mentioned above, we briefly describe an example (controller program and safety property) that expresses a bug that is impossible to occur in Kuai.

Control Message Reordering Bug. Let us consider a stateless firewall in Fig. 7a (controller is not shown), which is supposed to block incoming SSH packets from reaching the server (see [32] Appendix B-CP1). Formally, the safety property to be checked here is $\Box(\forall pkt \in S.rcvq\,.\,\neg pkt.\text{SSH})$. Initially, flow tables are empty. Switch A sends a *PacketIn* message to the controller when it receives the first packet from the client (as a result of a *nomatch* transition). The controller, in response to this request (and as a result of a *ctrl* transition), sends the following *FlowMod* messages to switch A; rule `r1` has the highest priority and drops all SSH packets, rule `r2` sends all packets from port 1 to port 2, and rule `r3` sends all packets from port 2 to port 1. If the packet that triggered the transition above is an SSH one, the controller drops it, otherwise, it instructs (through a *PacketOut* message) A to forward the packet to S. A bug-free controller should ensure that `r1` is installed before any other rule, therefore it must send a barrier request after the *FlowMod* message that contains `r1`. If, by mistake, the *FlowMod* message for `r2` is sent before the barrier request, A may install `r2` before `r1`, which will result in violating the given property. MOCS is able to capture this buggy behaviour as its semantics allows control messages prior to the barrier to be processed in a interleaved manner.

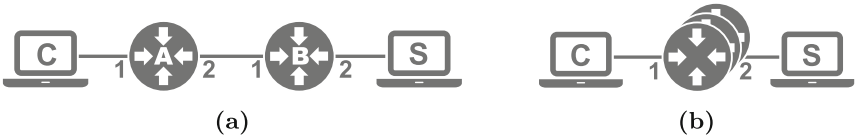


Fig. 7. Two networks with (a) two switches, and (b) n stateful firewall replicas

Wrong Nesting Level Bug. Consider a correct controller program that enforces that server S (Fig. 7a) is not accessible through SSH. Formally, the safety property to be checked here is $\Box(\forall pkt \in S.rcvq\,.\,\neg pkt.\text{SSH})$. For each incoming *PacketIn* message from switch A, it checks if the enclosed packet is an SSH one and destined to S. If not, it sends a *PacketOut* message instructing A to forward the packet to S. It also sends a *FlowMod* message to A with a rule that allows packets of the same protocol (not SSH) to reach S. In the opposite case (SSH), it checks (a Boolean flag) whether it had previously sent drop rules for SSH packets to the switches. If not, it sets flag to true, sends a *FlowMod* message with a rule

that drops SSH packets to A and drops the packet. Note that this inner block does not have an `else` statement.

A fairly common error is to write a statement at the wrong nesting level ([32] Appendix B-CP4). Such a mistake can be built into the above program by nesting the outer `else` branch in the inner `if` block, such that it is executed any time an SSH-packet is encountered but the SSH drop-rule has already been installed (i.e. flag `f` is true). Now, the SSH drop rule, once installed in switch A, disables immediately a potential $nomatch(A, p)$ with $p.\text{SSH} = true$ that would have sent packet p to the controller, but if it has not yet been installed, a second incoming SSH packet would lead to the execution of the `else` statement of the inner branch. This would violate the property defined above, as p will be forwarded to S[9].

MOCS can uncover this bug because of the correct modelling of the controller request queue and the asynchrony between the concurrent executions of control messages sent before a barrier. Otherwise, the second packet that triggers the execution of the wrong branch would not have appeared in the buffer before the first one had been dealt with by the controller. Furthermore, if all rules in messages up to a barrier were installed synchronously, the second packet would be dealt with correctly, so no bug could occur.

Inconsistent Update Bug. OpenFlow's barrier and barrier reply mechanisms allow for updating multiple network switches in a way that enables *consistent packet processing*, i.e., a packet cannot see a partially updated network where only a subset of switches have changed their forwarding policy in response to this packet (or any other event), while others have not done so. MOCS is expressive enough to capture this behaviour and related bugs. In the topology shown in Fig. 7a, let us assume that, by default, switch B drops all packets destined to S. Any attempt to reach S through A are examined separately by the controller and, when granted access, a relevant rule is installed at both switches (e.g. allowing all packets from C destined to S for given source and destination ports). Updates must be consistent, therefore the packet cannot be forwarded by A and dropped by B. Both switches must have the new rules in place, before the packet is forwarded. To do so, the controller, ([32] Appendix B-CP5), upon receiving a *PacketIn* message from the client's switch, sends the relevant rule to switch B (*FlowMod*) along with respective barrier (*BarrierReq*) and temporarily stores the packet that triggered this update. Only after receiving *BarrierRes* message from B, the controller will forward the previously stored packet back to A along with the relevant rule. This update is consistent and the packet is guaranteed to reach S. A (rather common) bug would be one where the controller installs the rules to both switches and at the same time forwards the packet to A. In this case, the packet may end up being dropped by B, if it arrives and gets processed before the relevant rule is installed, and therefore the invariant $\Box\big([drop(pkt, sw)]\,.\,\neg(pkt.dest = S)\big)$, where $[drop(pkt, sw)]$ is a quantifier that binds dropped packets (see definition in [32] Appendix B-CP5), would

[9] Here, we assume that the controller looks up a static forwarding table before sending *PacketOut* messages to switches.

be violated. For this example, it is crucial that MOCS supports barrier response messages.

5 Conclusion

We have shown that an OpenFlow compliant SDN model, with the right optimisations, can be model checked to discover subtle real-world bugs. We proved that MOCS can capture real-world bugs in a more complicated semantics without sacrificing performance.

But this is not the end of the line. One could automatically compute equivalence classes of packets that cover all behaviours (where we still computed manually). To what extent the size of the topology can be restricted to find bugs in a given controller is another interesting research question, as is the analysis of the number and length of interleavings necessary to detect certain bugs. In our examples, all bugs were found in less than a second.

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Software Verification

Code2Inv: A Deep Learning Framework for Program Verification

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Abstract. We propose a general end-to-end deep learning framework Code2Inv, which takes a verification task and a proof checker as input, and automatically learns a valid proof for the verification task by interacting with the given checker. Code2Inv is parameterized with an embedding module and a grammar: the former encodes the verification task into numeric vectors while the latter describes the format of solutions Code2Inv should produce. We demonstrate the flexibility of Code2Inv by means of two small-scale yet expressive instances: a loop invariant synthesizer for C programs, and a Constrained Horn Clause (CHC) solver.

1 Introduction

A central challenge in automating program verification lies in effective proof search. Counterexample-guided Inductive Synthesis (CEGIS) [3,4,17,31,32] has emerged as a promising paradigm for solving this problem. In this paradigm, a *generator* proposes a candidate solution, and a *checker* determines whether the solution is correct or not; in the latter case, the checker provides a counterexample to the generator, and the process repeats.

Finding loop invariants is arguably the most crucial part of proof search in program verification. Recent works [2,9,10,26,29,38] have instantiated the CEGIS paradigm for synthesizing loop invariants. Since *checking* loop invariants is a relatively standard process, these works target *generating* loop invariants using various approaches, such as stochastic sampling [29], syntax-guided enumeration [2,26], and decision trees with templates [9,10] or linear classifiers [38]. Despite having greatly advanced the state-of-the-art in program verification, however, there remains significant room for improvement in practice.

We set out to build a CEGIS-based program verification framework and identified five key objectives that it must address to be useful:

– The proof search should automatically evolve according to a given verification task as opposed to using exhaustive enumeration or a fixed set of search heuristics common in existing approaches.

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- The framework should be able to transfer knowledge across programs, that is, past runs should boost performance on similar programs in the future, which is especially relevant for CI/CD settings [15,20,25].
- The framework should be able to adapt to generate different kinds of invariants (e.g. non-linear or with quantifiers) beyond linear invariants predominantly targeted by existing approaches.
- The framework should be extensible to a new domain (e.g. constraint solving-based) by simply switching the underlying checker.
- The generated invariants should be natural, e.g. avoid overfitting due to human-induced biases in the proof search heuristic or invariant structure commonly imposed through templates.

We present Code2Inv, an end-to-end deep learning framework which aims to realize the above objectives. Code2Inv has two key differences compared to existing CEGIS-based approaches. First, instead of simply focusing on counterexamples but ignoring program structure, Code2Inv learns a neural representation of program structure by leveraging graph neural networks [8,11,19,28], which enable to capture structural information and thereby generalize to different but structurally similar programs. Secondly, Code2Inv reduces loop invariant generation into a deep reinforcement learning problem [22,34]. No search heuristics or training labels are needed from human experts; instead, a neural policy for loop invariant generation can be automatically learned by interacting with the given proof checker on the fly. The learnable neural policy generates a loop invariant by taking a sequence of actions, which can be flexibly controlled by a grammar that defines the structure of loop invariants. This decoupling of the action definition from policy learning enables Code2Inv to adapt to different loop invariants or other reasoning tasks in a new domain with almost no changes except for adjusting the grammar or the underlying checker.

We summarize our contributions as follows:

- We present a framework for program verification, Code2Inv, which leverages deep learning and reinforcement learning through the use of graph neural network, tree-structured long short-term memory network, attention mechanism, and policy gradient.
- We show two small-scale yet expressive instances of Code2Inv: a loop invariant synthesizer for C programs and a Constrained Horn Clause (CHC) solver.
- We evaluate Code2Inv on a suite of 133 C programs from SyGuS [2] by comparing its performance with three state-of-the-art approaches and showing that the learned neural policy can be transferred to similar programs.
- We perform two case studies showing the flexibility of Code2Inv on different classes of loop invariants. We also perform a case study on the naturalness of the loop invariants generated by various approaches.

2 Background

In this section, we introduce artificial neural network concepts used by Code2Inv. A multilayer perceptron (MLP) is a basic neural network model which can

approximate an arbitrary continuous function $\mathbf{y} = f^*(\mathbf{x})$, where $\mathbf{x}$ and $\mathbf{y}$ are numeric vectors. An MLP defines a mapping $\mathbf{y} = f(\mathbf{x}; \theta)$, where θ denotes weights of connections, which are usually trained using gradient descent methods.

Recurrent neural networks (RNNs) approximate the mapping from a sequence of inputs $\mathbf{x}^{(1)}, ..., \mathbf{x}^{(t)}$ to either a single output $\mathbf{y}$ or a sequence of outputs $\mathbf{y}^{(1)}, ..., \mathbf{y}^{(t)}$. An RNN defines a mapping $\mathbf{h}^{(t)} = f(\mathbf{h}^{(t-1)}, \mathbf{x}^{(t)}; \theta)$, where $\mathbf{h}^{(t)}$ is the hidden state, from which the final output $\mathbf{y}^{(t)}$ can be computed (e.g. by a non-linear transformation or an MLP). A common RNN model is the long short-term memory network (LSTM) [16] which is used to learn long-term dependencies. Two common variants of LSTM are gated recurrent units (GRUs) [7] and tree-structured LSTM (Tree-LSTM) [35]. The former simplifies the LSTM for efficiency while the latter extends the modeling ability to tree structures.

In many domains, graphs are used to represent data with rich structure, such as programs, molecules, social networks, and knowledge bases. Graph neural networks (GNNs) [1,8,11,19,36] are commonly used to learn over graph-structured data. A GNN learns an embedding (i.e. real-valued vector) for each node of the given graph using a recursive neighborhood aggregation (or neural message passing) procedure. After training, a node embedding captures the structural information within the node's K-hop neighborhood, where K is a hyper-parameter. A simple aggregation of all node embeddings or pooling [37] according to the graph structure summarizes the entire graph into an embedding. GNNs are parametrized with other models such as MLPs, which are the learnable non-linear transformations used in message passing, and GRUs, which are used to update the node embedding.

Lastly, the generalization ability of neural networks can be improved by an external memory [12,13,33] which can be accessed using a differentiable *attention mechanism* [5]. Given a set of neural embeddings, which form the external memory, an attention mechanism assigns a likelihood to each embedding, under a given neural context. These likelihoods guide the selection of decisions that are represented by the chosen embeddings.

3 Framework

We first describe the general framework, Code2Inv, and then illustrate two instances, namely, a loop invariant synthesizer for C programs and a CHC solver.

Figure 1 defines the domains of program structures and neural structures used in Code2Inv. The framework is parameterized by graph constructors $\mathcal{G}$ that produce graph representations of verification instance T and invariant grammar A, denoted G_{inst} and G_{inv}, respectively. The invariant grammar uses placeholder symbols H, which represent *abstract* values of entities such as variables, constants, and operators, and will be replaced by *concrete* values from the verification instance during invariant generation. The framework requires a black-box function *check* that takes a verification instance T and a candidate invariant *inv*, and returns success (denoted $\perp$) or a counterexample *cex*.

Domains of Program Structures:

$$
\begin{array}{rcll}
\boldsymbol{\mathcal{G}}(T) & = & G_{\text{inst}} & (G_{\text{inst}} \text{ is graph representation of } \textit{verification instance } T) \\
\boldsymbol{\mathcal{G}}(A) & = & G_{\text{inv}} & (G_{\text{inv}} \text{ is graph representation of } \textit{invariant grammar } A) \\
A & = & \langle \Sigma \uplus H, N, P, S \rangle & \text{(invariant grammar)} \\
x & \in & H \uplus N & \text{(set of placeholder symbols and non-terminals)} \\
v & \in & \Sigma & \text{(set of terminals)} \\
n & \in & N & \text{(set of non-terminals)} \\
p & \in & P & \text{(production rule)} \\
 & & S & \text{(start symbol)} \\
inv & \in & \boldsymbol{\mathcal{L}}(A) & \text{(invariant candidate)} \\
cex & \in & \mathbb{C} & \text{(counterexample)} \\
C & \in & \boldsymbol{\mathcal{P}}(\mathbb{C}) & \text{(set of counterexamples)} \\
check(T, inv) & \in & \{\bot\} \uplus \mathbb{C} & \text{(invariant validation)}
\end{array}
$$

Domains of Neural Structures:

$$
\begin{array}{rcll}
\pi & = & \langle \nu_{\text{T}}, \nu_{\text{A}}, \eta_{\text{T}}, \eta_{\text{A}}, \alpha_{\text{ctx}}, \epsilon_{\text{inv}} \rangle & \text{(neural policy)} \\
d & & & \text{(positive integer size of embedding)} \\
\nu_{\text{T}},\ \eta_{\text{T}}(G_{\text{inst}}) & \in & \mathbb{R}^{|G_{\text{inst}}| \times d} & \text{(graph embedding of verification instance)} \\
\nu_{\text{A}},\ \eta_{\text{A}}(G_{\text{inv}}) & \in & \mathbb{R}^{|G_{\text{inv}}| \times d} & \text{(graph embedding of invariant grammar)} \\
ctx & \in & \mathbb{R}^d & \text{(neural context)} \\
state & \in & \mathbb{R}^d & \text{(partially generated invariant state)} \\
\alpha_{\text{ctx}} & \in & \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d & \text{(attention context)} \\
\epsilon_{\text{inv}} & \in & \boldsymbol{\mathcal{L}}(A) \to \mathbb{R}^d & \text{(invariant encoder)} \\
aggregate & \in & \mathbb{R}^{\text{k} \times d} \to \mathbb{R}^d & \text{(aggregation of embeddings)} \\
\nu_{\text{A}}[n] & \in & \mathbb{R}^{\text{k} \times d} & \text{(embedding of production rules for non-terminal } n\text{,} \\
 & & & \text{where k is number of production rules of } n \text{ in } G_{\text{inv}}) \\
\nu_{\text{T}}[h] & \in & \mathbb{R}^{\text{k} \times d} & \text{(embedding of nodes annotated by placeholder } h\text{,} \\
 & & & \text{where k is number of nodes annotated by } h \text{ in } G_{\text{inst}})
\end{array}
$$

Fig. 1. Semantic domains. $\boldsymbol{\mathcal{L}}(A)$ denotes the set of all sentential forms of A.

The key component of the framework is a neural policy π which comprises four neural networks. Two graph neural networks, η_{T} and η_{A}, are used to compute neural embeddings, ν_{T} and ν_{A}, for graph representations G_{inst} and G_{inv}, respectively. The neural network α_{ctx}, implemented as a GRU, maintains the attention context *ctx* which controls the selection of the production rule to apply or the concrete value to replace a placeholder symbol at each step of invariant generation. The neural network ϵ_{inv}, implemented as a Tree-LSTM, encodes the partially generated invariant into a numeric vector denoted *state*, which captures the state of the generation that is used to update the attention context *ctx*.

Algorithm 1 depicts the main algorithm underlying Code2Inv. It takes a verification instance and a proof checker as input and produces an invariant that suffices to verify the given instance[1]. At a high level, Code2Inv learns a neural policy, in lines 1–5. The algorithm first initializes the neural policy and the set of counterexamples (line 1–2). The algorithm then iteratively samples a candidate invariant (line 4) and improves the policy using a reward for the new

[1] Fuzzers may be applied first so that the confidence of existence of a proof is high.

Algorithm 1. Code2Inv Framework

Input: a verification instance T and a proof checker *check*
Output: a invariant *inv* satisfying $check(T, inv) = \bot$
Parameter: graph constructor $\mathcal{G}$ and invariant grammar A

$\pi \leftarrow$ `initPolicy(`T, A`)`
$C \leftarrow \emptyset$
while *true* **do**
  $inv \leftarrow$ `sample(`π, T, A`)`
  $\langle \pi, C \rangle \leftarrow$`improve(`$\pi, inv, C$`)`

Function `initPolicy(`T, A`)`
  Initialize weights of $\eta_{\mathrm{T}}, \eta_{\mathrm{A}}, \alpha_{\mathrm{ctx}}, \epsilon_{\mathrm{inv}}$ with random values
  $\nu_{\mathrm{T}} \leftarrow \eta_{\mathrm{T}}(\mathcal{G}(T))$
  $\nu_{\mathrm{A}} \leftarrow \eta_{\mathrm{A}}(\mathcal{G}(A))$
  return $\langle \nu_{\mathrm{T}}, \nu_{\mathrm{A}}, \eta_{\mathrm{T}}, \eta_{\mathrm{A}}, \alpha_{\mathrm{ctx}}, \epsilon_{\mathrm{inv}} \rangle$

Function `sample(`π, T, A`)`
  $inv \leftarrow A.\mathrm{S}$
  $ctx \leftarrow aggregate(\pi.\nu_{\mathrm{T}})$
  while *inv* is partially derived **do**
    $x \leftarrow$ leftmost non-terminal or placeholder symbol in *inv*
    $state \leftarrow \pi.\epsilon_{\mathrm{inv}}(inv)$
    $ctx \leftarrow \pi.\alpha_{\mathrm{ctx}}(ctx, state)$
    if x is non-terminal **then**
      $p \leftarrow$ `attention(`$ctx, \pi.\nu_{\mathrm{A}}[x], \mathcal{G}(A)$`)`
      expand *inv* according to p
    else
      $v \leftarrow$ `attention(`$ctx, \pi.\nu_{\mathrm{T}}[x], \mathcal{G}(T)$`)`
      replace x in *inv* with v
  return *inv*

Function `improve(`π, inv, C`)`
  $n \leftarrow$ number of counter-examples C that *inv* can satisfy
  if $n = |C|$ **then**
    $cex \leftarrow check(T, inv)$
    if $cex = \bot$ **then**
      save *inv* and weights of π
      exit `// a sufficient invariant is found`
    else
      $C \leftarrow C \cup \{cex\}$
  $r \leftarrow n/|C|$
  $\pi \leftarrow$ `updatePolicy(`π, r`)`
  return $\langle \pi, C \rangle$

Function `updatePolicy(`π, r`)`
  Update weights of $\pi.\eta_{\mathrm{T}}, \pi.\eta_{\mathrm{A}}, \pi.\alpha_{\mathrm{ctx}}, \pi.\epsilon_{\mathrm{inv}}, \pi.\nu_{\mathrm{T}}, \pi.\nu_{\mathrm{A}}$ by
  standard policy gradient [34] using reward r

Function `attention(`ctx, ν, G`)`
  Return node t in G such that dot product of ctx and $\nu[t]$
  is maximum over all nodes of G

candidate based on the accumulated counterexamples (line 5). We next elucidate upon the initialization, policy sampling, and policy improvement procedures.

Initialization. The `initPolicy` procedure (line 6–10) initializes the neural policy. All four neural networks are initialized with random weights (line 7), and graph embeddings $\nu_{\mathrm{T}}, \nu_{\mathrm{A}}$ for verification task T and invariant grammar A are computed by applying corresponding graph neural networks $\eta_{\mathrm{T}}, \eta_{\mathrm{A}}$ to their graph representations $\boldsymbol{\mathcal{G}}(T), \boldsymbol{\mathcal{G}}(A)$ respectively. Alternatively, the neural networks can be initialized with pre-trained weights, which can boost overall performance.

Neural Policy Sampling. The `sample` procedure (lines 11–24) generates a candidate invariant by executing the current neural policy. The candidate is first initialized to the start symbol of the given grammar (line 12), and then updated iteratively (lines 14–23) until it is complete (i.e. there are no non-terminals). Specifically, the candidate is updated by either expanding its leftmost non-terminal according to one of its production rules (lines 19–20) or by replacing its leftmost placeholder symbol with some concrete value from the verification instance (lines 22–23). The selection of a production rule or concrete value is done through an *attention mechanism*, which picks the most likely one according to the current context and corresponding region of external memory. The neural context is initialized to the aggregation of embeddings of the given verification instance (line 13), and then maintained by α_{ctx} (line 17) which, at each step, incorporates the neural state of the partially generated candidate invariant (line 16), where the neural state is encoded by ϵ_{inv}.

Neural Policy Improvement. The `improve` procedure (lines 25–36) improves the current policy by means of a *continuous* reward. Simply checking whether the current candidate invariant is sufficient or not yields a discrete reward of 1 (yes) or 0 (no). This reward is too sparse to improve the policy, since most candidate invariants generated are insufficient, thereby almost always yielding a zero reward. Code2Inv addresses this problem by accumulating counterexamples provided by the checker. Whenever a new candidate invariant is generated, Code2Inv tests the number of counterexamples it can satisfy (line 26), and uses the fraction of satisfied counterexamples as the reward (line 34). If all counterexamples are satisfied, Code2Inv queries the checker to validate the candidate (line 28). If the candidate is accepted by the checker, then a sufficient invariant was found, and the learned weights of the neural networks are saved for speeding up similar verification instances in the future (lines 29–31). Otherwise, a new counterexample is accumulated (line 33). Finally, the neural policy (including the neural embeddings) is updated based on the reward.

Framework Instantiations. We next show two instantiations of Code2Inv by customizing the graph constructor $\boldsymbol{\mathcal{G}}$. Specifically, we demonstrate two scenarios of graph construction: 1) by carefully exploiting task specific knowledge, and 2) with minimum information of the given task.

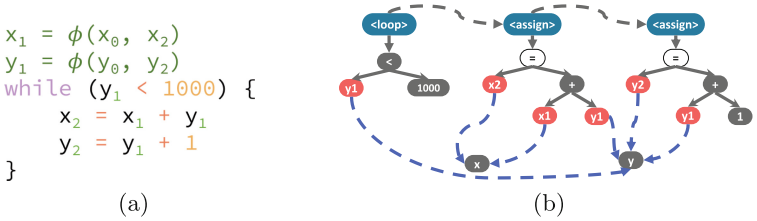


Fig. 2. (a) C program snippet in SSA form; (b) its graph representation.

Instantiation to Synthesize Loop Invariants for C Programs. An effective graph representation for a C program should reflect its control-flow and data-flow information. We leverage the static single assignment (SSA) transformation for this purpose. Figure 2 illustrates the graph construction process. Given a C program, we first apply SSA transformation as shown in Fig. 2a, from which a graph is constructed as shown in Fig. 2b. The graph is essentially abstract syntax trees (ASTs) augmented with control-flow (black dashed) edges and data-flow (blue dashed) edges. Different types of edges will be modeled as different message passing channels used in graph neural networks so that rich structural information can be captured more effectively by the neural embeddings. Furthermore, certain nodes (marked black) are annotated with placeholder symbols and will be used to fill corresponding placeholders during invariant generation. For instance, variables `x` and `y` are annotated with `VAR`, integer values `1000` and `1` are annotated with `CONST`, and the operator `<` is annotated with `OP`.

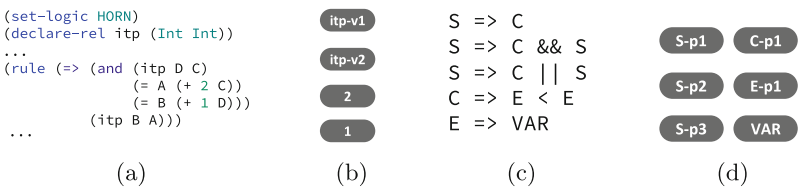


Fig. 3. (a) CHC instance snippet; (b) node representation for the CHC example; (c) example of invariant grammar; (d) node representation for the grammar.

Instantiation to Solve Constrained Horn Clauses (CHC). CHC are a uniform way to represent recursive, inter-procedural, and multi-threaded programs, and serve as a suitable basis for automatic program verification [6] and refinement type inference [21]. Solving a CHC instance involves determining unknown predicates that satisfy a set of logical constraints. Figure 3a shows a simple example of a CHC instance where *itp* is the unknown predicate. It is easy to see that *itp* in fact represents an invariant of a loop. Thus, CHC solving can be viewed as a generalization of finding loop invariants [6].

Unlike C programs, which have explicit control-flow and data-flow information, a CHC instance is a set of *un-ordered* Horn rules. The graph construction for Horn rules is not as obvious as for C programs. Therefore, instead of deliberately constructing a graph that incorporates detailed domain-specific information, we use a *node representation*, which is a degenerate case of graph representation and requires only necessary nodes but no edges. Figure 3b shows the node representation for the CHC example from Fig. 3a. The top two nodes are derived from the signature of unknown predicate *itp* and represent the first and the second arguments of *itp*. The bottom two nodes are constants extracted from the Horn rule. We empirically show that node representation works reasonably well. The downside of node representation is that no structural information is captured by the neural embeddings which in turn prevents the learned neural policy from generalizing to other structurally similar instances.

Embedding Invariant Grammar. Lastly, both instantiations must define the embedding of the invariant grammar. The grammar can be arbitrarily defined, and similar to CHCs, there is no obvious information such as control- or data-flow to leverage. Thus, we use node representation for the invariant grammar as well. Figure 3c and Fig. 3d shows an example of invariant grammar and its node representation, respectively. Each node in the graph represents either a terminal or a production rule for a non-terminal. Note that this representation does not prevent the neural policy from generalizing to similar instances as long as they share the same invariant grammar. This is feasible because the invariant grammar does not contain instance specific details, which are abstracted away by placeholder symbols like `VAR`, `CONST`, and `OP`.

4 Evaluation

We first discuss the implementation, particularly the improvement over our previous prototype [30], and then evaluate our framework in a number of aspects, such as performance, transferability, flexibility, and naturalness.

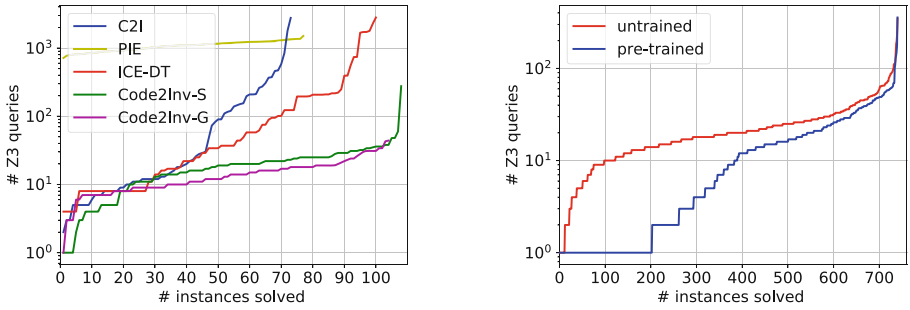
Implementation. Code2Inv[2] consists of a frontend, which converts an instance into a graph, and a backend, which maintains all neural components (i.e. neural embeddings and policy) and interacts with a checker. Our previous prototype has a very limited frontend based on CIL [24] and no notion of invariant grammar in the backend. We made significant improvements in both the frontend and the backend. We re-implemented the frontend for C programs based on Clang and implemented a new frontend for CHCs. We also re-implemented the backend to accept a configurable invariant grammar. Furthermore, we developed a standard graph format, which decouples the frontend and backend, and a clean interface between the backend and the checker. No changes are needed in the backend to support new instantiations.

Evaluation Setup. We evaluate both instantiations of Code2Inv by comparing each instantiation with corresponding state-of-the-art solvers. For the task of

[2] Our artifacts are available on GitHub: https://github.com/PL-ML/code2inv.

synthesizing loop invariants for C programs, we use the same suite of benchmarks from our previous work [30], which consists of 133 C programs from SyGuS [2]. We compare Code2Inv with our previous specialized prototype and three other state-of-the-art verification tools: C2I [29], LoopInvGen [26] and ICE-DT [10]. For the CHC solving task, we collect 120 CHC instances using SeaHorn [14] to reduce the C benchmark programs into CHCs.[3] We compare Code2Inv with two state-of-the-art CHC solvers: Spacer [18], which is the default fixedpoint engine of Z3, and LinearyArbitrary [38]. We run all solvers on a single 2.4 GHz AMD CPU core up to 12 h and using up to 4 GB memory. Unless specified otherwise, Code2Inv is always initialized randomly, that is, untrained.

Performance. Given that both the hardware and the software environments could affect the absolute running time and that all solvers for loop invariant generation for C programs rely on the same underlying SMT engine, Z3 [23], we compare the performance in terms of number of Z3 queries. We note that this is an imperfect metric but a relatively objective one that also highlights salient features of Code2Inv. Figure 4a shows the plot of verification cost (i.e. number of Z3 queries) by each solver and the number of C programs successfully verified within the corresponding cost. Code2Inv significantly outperforms other state-of-the-art solvers in terms of verification cost and the general framework Code2Inv-G achieves performance comparable to (slightly better than) the previous specialized prototype Code2Inv-S.



(a) (b)

Fig. 4. (a) Comparison of Code2Inv with state-of-the-art solvers; (b) comparison between untrained model and pre-trained model.

Transferability. Another hallmark of Code2Inv is that, along with the desired loop invariant, it also learns a neural policy. To evaluate the performance benefits of the learned policy, we randomly perturb the C benchmark programs by various edits (e.g. renaming existing variables and injecting new variables and

[3] SeaHorn produces empty Horn rules on 13 (out of 133) C programs due to optimizations during VC generation that result in proving the assertions of interest.

statements). For each program, we obtain 100 variants, and use 90 for training and 10 for testing. Figure 4b shows the performance difference between the untrained model (i.e. initialized with random weights) and the pre-trained model (i.e. initialized with pre-trained weights). Our results indicate that the learned neural policy can be transferred to accelerate the search for loop invariants for similar programs. This is especially useful in the CI/CD setting [25] where programs evolve incrementally and quick turnaround time is indispensable.

Flexibility. Code2Inv can be instantiated or extended in a very flexible manner. For one instance, with a simple frontend (e.g. node representation as discussed above), Code2Inv can be customized as a CHC solver. Our evaluation shows that, without any prior knowledge about Horn rules, Code2Inv can solve 94 (out of 120) CHC instances. Although it is not on a par with state-of-the-art CHC solvers Spacer and LinearArbitrary, which solve 112 and 118 instances, respectively, Code2Inv provides new insights for solving CHCs and could be further improved by better embeddings and reward design.

As another example, by simply adjusting the invariant grammar, Code2Inv is immediately ready for solving CHC tasks involving *non-linear* arithmetic. Our case study shows that Code2Inv successfully solves 5 (out of 7) non-linear instances we created[4], while both Spacer and LinearArbitrary failed to solve any of them. Tasks involving non-linear arithmetic are particularly challenging because the underlying checker is more likely to get stuck, and no feedback (e.g. counterexample) can be provided, which is critical for existing solvers like Spacer and LinearArbitrary to make progress. This highlights another strength of Code2Inv—even if the checker gets stuck, the learning process can still continue by simply assigning zero or negative reward.

```
Solution found by Spacer:
(and (or (not (<= B 16)) (not (>= A 8)))
         (not (<= B 0))
     (or (not (<= B 2)) (<= A 0))
     (or (not (<= B 4)) (not (>= A 2)))
     (or (not (<= B 6)) (not (>= A 3)))
     (or (not (<= B 8)) (not (>= A 4)))
     (or (not (<= B 10)) (not (>= A 5)))
     (or (not (<= B 12)) (not (>= A 6)))
     (or (not (<= B 14)) (not (>= A 7)))))))

Code2Inv: (<= v0 (- v1 v0))
```

(a) Spacer on add2.smt

```
Solution found by LinearArbitrary:
(or
  (and true !(V0<=-50)
           V1<=5  ((1*V0)+(-1*V1))<=-45
           V1<=4  !(((1*V0)+(-1*V1))<=-51)
          !(V1<=2)!(((1*V0)+(-1*V1))<=-50)
          !(V1<=3) ((1*V0)+(1*V1))<=-40
  )
  ... // omitting other 4 similar (and ...)
)

Code2Inv: (or (< V0 (+ 0 0)) (> V1 V0))
```

(b) LinearArbitrary on 84.c.smt

Fig. 5. Comparison of solution naturalness.

Naturalness. Our final case study concerns the naturalness of solutions. As illustrated in Fig. 5, solutions discovered by Code2Inv tend to be more natural, whereas Spacer and LinearArbitrary tend to find solutions that unnecessarily depend on constants from the given verification instance. Such *overfitted* solutions may become invalid when these constants change. Note that

[4] The non-linear instances we created are available in the artifact.

expressions such as `(+ 0 0)` in Code2Inv's solutions can be eliminated by post-processing simplification akin to peephole optimization in compilers. Alternatively, the reward mechanism in Code2Inv could incorporate a regularizer on the naturalness.

Limitations. Code2Inv does not support finding loop invariants for programs with multiple loops, function calls, or recursion. Code2Inv generally runs slower compared to other contemporary approaches. Specifically, 90% of the solved C instances took 2 h or less, and the rest could take up to 12 hours to solve. This could be improved upon by leveraging GPUs, developing more efficient training algorithms, or leveraging templates [27].

5 Conclusion

We presented a framework Code2Inv which automatically learns invariants (or more generally unknown predicates) by interacting with a proof checker. Code2Inv is a general and learnable tool for solving many different verification tasks and can be flexibly configured with a grammar and a graph constructor. We compared its performance with state-of-the-art solvers for both C programs and CHC formulae, and showed that it can adapt to different types of inputs with minor changes. We also showed, by simply varying the input grammar, how it can tackle non-linear invariant problems which other solvers are not equipped to work with, while still giving results that are relatively natural to read.

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MetaVal: Witness Validation via Verification

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Abstract. Witness validation is an important technique to increase trust in verification results, by making descriptions of error paths (violation witnesses) and important parts of the correctness proof (correctness witnesses) available in an exchangeable format. This way, the verification result can be validated independently from the verification in a second step. The problem is that there are unfortunately not many tools available for witness-based validation of verification results. We contribute to closing this gap with the approach of *validation via verification*, which is a way to automatically construct a set of validators from a set of existing verification engines. The idea is to take as input a specification, a program, and a verification witness, and produce a new specification and a transformed version of the original program such that the transformed program satisfies the new specification if the witness is useful to confirm the result of the verification. Then, an 'off-the-shelf' verifier can be used to validate the previously computed result (as witnessed by the verification witness) via an ordinary verification task. We have implemented our approach in the validator MetaVal, and it was successfully used in SV-COMP 2020 and confirmed 3 653 violation witnesses and 16 376 correctness witnesses. The results show that MetaVal improves the effectiveness (167 uniquely confirmed violation witnesses and 833 uniquely confirmed correctness witnesses) of the overall validation process, on a large benchmark set. All components and experimental data are publicly available.

Keywords: Computer-aided verification · Software verification · Program analysis · Software model checking · Certification · Verification witnesses · Validation of verification results · Reducer

1 Introduction

Formal software verification becomes more and more important in the development process for software systems of all types. There are many verification tools available to perform verification [4]. One of the open problems that was addressed only recently is the topic of results validation [10–12,37]: The verification work is often done by untrusted verification engines, on untrusted computing infrastructure, or even on approximating computation systems, and static-analysis tools suffer from false positives that engineers in practice hate because they are tedious to refute [20]. Therefore, it is necessary to validate verification results,

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ideally by an independent verification engine that likely does not have the same weaknesses as the original verifier. Witnesses also help serving as an interface to the verification engine, in order to overcome integration problems [1].

The idea to witness the correctness of a program by annotating it with assertions is as old as programming [38], and from the beginning of model checking it was felt necessary to witness counterexamples [21]. Certifying algorithms [30] are not only computing a solution but also produce a witness that can be used by a computationally much less expensive checker to (re-)establish the correctness of the solution. In software verification, witnesses became standardized[1] and exchangeable about five years ago [10,11]. In the meanwhile, the exchangeable witnesses can be used also for deriving tests from witnesses [12], such that an engineer can study an error report additionally with a debugger. The ultimate goal of this direction of research is to obtain witnesses that are certificates and can be checked by a fully trusted validator based on trusted theorem provers, such as Coq and Isabelle, as done already for computational models that are 'easier' than C programs [40].

Yet, although considered very useful, there are not many witness validators available. For example, the most recent competition on software verification (SV-COMP 2020)[2] showcases 28 software verifiers but only 6 witness validators. Two were published in 2015 [11], two more in 2018 [12], the fifth in 2020 [37], and the sixth is MetaVal, which we describe here. Witness validation is an interesting problem to work on, and there is a large, yet unexplored field of opportunities. It involves many different techniques from program analysis and model checking. However, it seems that this also requires a lot of engineering effort.

Our solution *validation via verification* is a construction that takes as input an off-the-shelf software verifier and a new program transformer, and composes a witness validator in the following way (see Fig. 1): First, the transformer takes the original input program and transforms it into a new program. In case of a violation witness, which describes a path through the program to a specific program location, we transform the program such that all parts that are marked as unnecessary for the path by the witness are pruned. This is similar to the reducer for a condition in reducer-based conditional model checking [14]. In case of a correctness witness, which describes invariants that can be used in a correctness proof, we transform the program such that the invariants are asserted (to check that they really hold) and assumed (to use them in a re-constructed correctness proof). A standard verification engine is then asked to verify that (1) the transformed program contains a feasible path that violates the original specification (violation witness) or (2) the transformed program satisfies the original specification and all assertions added to the program hold (correctness witness).

MetaVal is an implementation of this concept. It performs the transformation according to the witness type and specification, and can be configured to use any of the available software verifiers[3] as verification backend.

[1] Latest version of standardized witness format: https://github.com/sosy-lab/sv-witnesses
[2] https://sv-comp.sosy-lab.org/2020/systems.php
[3] https://gitlab.com/sosy-lab/sv-comp/archives-2020/tree/master/2020

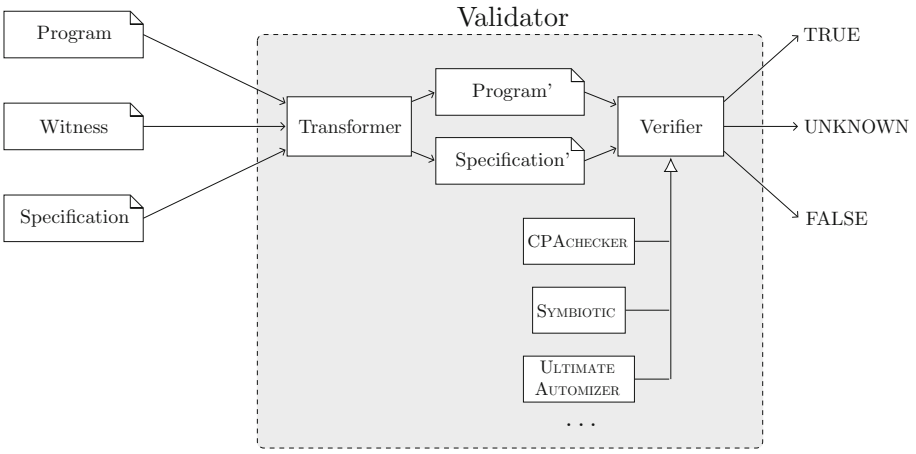

Fig. 1. Validator construction using readily available verifiers

Contributions. MetaVal contributes several important benefits:

- The program transformer was a one-time effort and is available from now on.
- Any existing standard verifier can be used as verification backend.
- Once a new verification technology becomes available in a verification tool, it can immediately be turned into a validator using our new construction.
- Technology bias can be avoided by complementing the verifier by a validator that is based on a different technology.
- Selecting the strongest verifiers (e.g., by looking at competition results) can lead to strong validators.
- All data and software that we describe are publicly available (see Sect. 6).

2 Preliminaries

For the theoretical part, we will have to set a common ground for the concepts of verification witnesses [10,11] as well as reducers [14]. In both cases, programs are represented as control-flow automata (CFAs). A *control-flow automaton* $C = (L, l_0, G)$ consists of a set L of control locations, an initial location $l_0 \in L$, and a set $G \subseteq L \times Ops \times L$ of control-flow edges that are labeled with the operations in the program. In the mentioned literature on witnesses and reducers, a simple programming language is used in which operations are either assignments or assumptions over integer variables. Operations $op \in Ops$ in such a language can be represented by formulas in first order logic over the sets V,V' of program variables before and after the transition, which we denote by $op(V, V')$. In order to simplify our construction later on, we will also allow mixed operations of the form $f(V) \wedge (x' = g(V))$ that combine assumptions with an assignment, which would otherwise be represented as an assumption followed by an assignment operation.

```
1   void fun(uint x, uint y, uint z) {
2     if (x > y) {
3       z = 2*x-y;
4     } else {
5       z = 2*y-x+1;
6     }
7     if (z>y || z>x) {
8       return;
9     } else {
10      error();
11    }
12  }
```

Fig. 2. Example program for both correctness and violation witness validation

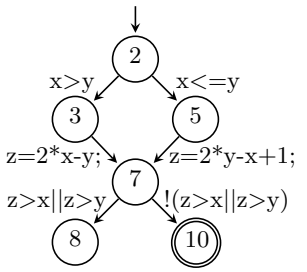

Fig. 3. CFA C of example program from Fig. 2

The conversion from the source code into a CFA and vice versa is straight forward, provided that the CFA is deterministic. A CFA is called *deterministic* if in case there are multiple outgoing CFA edges from a location l, the assumptions in those edges are mutually exclusive (but not necessarily exhaustive).

Since our goal is to validate (i.e., prove or falsify) the statement that a program fulfills a certain specification, we need to additionally model the property to be verified. For properties that can be translated into non-reachability, this can be done by defining a set $T \subseteq L$ of target locations that shall not be reached. For the example program in Fig. 2 we want to verify that the call in line 10 is not reachable. In the corresponding CFA in Fig. 3 this is represented by the reachability of the location labeled with 10. Depending on whether or not a verifier accounts for the overflow in this example program, it will either consider the program safe or unsafe, which makes it a perfect example that can be used to illustrate both correctness and violation witnesses.

In order to reason about the soundness of our approach, we need to also formalize the program semantics. This is done using the concept of concrete data states. A *concrete data state* is a mapping from the set V of program variables to their domain $\mathbb{Z}$, and a *concrete state* is a pair of control location and concrete data state. A *concrete program path* is then defined as a sequence $\pi = (c_0, l_0) \xrightarrow{g_1} \ldots \xrightarrow{g_n} (c_n, l_n)$ where c_0 is the initial concrete data state, $g_i = (l_{i-1}, op_i, l_i) \in G$, and $c_{i-1}(V), c_i(V') \vDash op_i$. A *concrete execution* $ex(\pi)$ is then derived from a path π by only looking at the sequence $(c_0, l_0) \ldots (c_n, l_n)$ of concrete states from the path. Note the we deviate here from the definition given in [14], where concrete executions do not contain information about the program locations. This is necessary here since we want to reason about the concrete executions that fulfill a given non-reachability specification, i.e., that never reach certain locations in the original program.

Witnesses are formalized using the concept of protocol automata [11]. A *protocol automaton* $W = (Q, \Sigma, \delta, q_0, F)$ consists of a set Q of states, a set of transition labels $\Sigma = 2^G \times \Phi$, a transition relation $\delta \subseteq Q \times \Sigma \times Q$, an initial state q_0, and a set $F \subseteq Q$ of final states. A state is a pair that consists of a name to identify

the state and a predicate over the program variables V to represent the state invariant.[4] A transition label is a pair that consists of a subset of control-flow edges and a predicate over the program variables V to represent the guard condition for the transition to be taken. An *observer automaton* [11,13,32,34,36] is a protocol automaton that does not restrict the state space, i.e., if for each state $q \in Q$ the disjunction of the guard conditions of all outgoing transitions is a tautology. Violation witnesses are represented by protocol automata in which all state invariants are *true*. Correctness witnesses are represented by observer automata in which the set of final states is empty.

3 Approach

3.1 From Witnesses to Programs

When given a CFA $C = (L, l_0, G)$, a specification $T \subseteq L$, and a witness automaton $W = (Q, \Sigma, \delta, q_0, F)$, we can construct a product automaton $A_{C \times W} = (L \times Q, (l_0, q_0), \Gamma, T \times F)$ where $\Gamma \subseteq (L \times Q) \times (Ops \times \Phi) \times (L \times Q)$. The new transition relation Γ is defined by allowing for each transition g in the CFA only those transitions (S, φ) from the witness where $g \in S$ holds:

$$\Gamma = \left\{ \left((l_i, q_i), (op, \varphi), (l_j, q_j) \right) \mid \exists S : \left(q_i, (S, \varphi), q_j \right) \in \delta, (l_i, op, l_j) \in S \right\}$$

We can now define the semantics of a witness by looking at the paths in the product automaton and mapping them to concrete executions in the original program. A path of the product automaton $A_{C,W}$ is a sequence $(l_0, q_0) \xrightarrow{\alpha_0} \ldots \xrightarrow{\alpha_{n-1}} (l_n, q_n)$ such that $\left((l_i, q_i), \alpha_i, (l_{i+1}, q_{i+1}) \right) \in \Gamma$ and $\alpha_i = (op_i, \phi_i)$.

It is evident that the automaton $A_{C \times W}$ can easily be mapped to a new program $C_{C \times W}$ by reducing the pair (op, φ) in its transition relation to an operation $\overline{op}$. In case op is a pure assumption of the form $f(V)$ then $\overline{op}$ will simply be $f(V) \wedge \varphi(V)$. If op is an assignment of the form $f(V) \wedge (x' = g(V))$, then $\overline{op}$ will be $(f(V) \wedge \varphi(V)) \wedge (x' = g(V))$. This construction has the drawback that the resulting CFA might be non-deterministic, but this is actually not a problem when the corresponding program is only used for verification. The non-determinism can be expressed in the source code by using non-deterministic values, which are already formalized by the community and established in the SV-COMP rules, and therefore also supported by all participating verifiers. The concrete executions of $C_{C \times W}$ can be identified with concrete executions of C by projecting their pairs (l, q) on their first element. Let $proj_C(ex(C_{C \times W}))$ denote the set of concrete executions that is derived this way. Due to how the relation Γ of $A_{C \times W}$ is constructed, it is guaranteed that this is a subset of the executions of C, i.e., $proj_C(ex(C_{C \times W})) \subseteq ex(C)$. In this respect the witness acts in very much the same way as a reducer [14], and the reduction of the search space is also one of the desired properties of a validator for violation witnesses.

[4] These invariants are the central piece of information in correctness witnesses. While invariants that proof a program correct can be hard to come up with, they are usually easier to check.

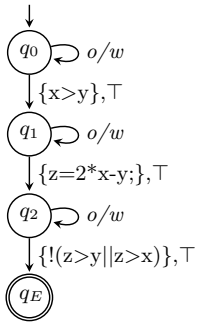

Fig. 4. Violation witness W_V

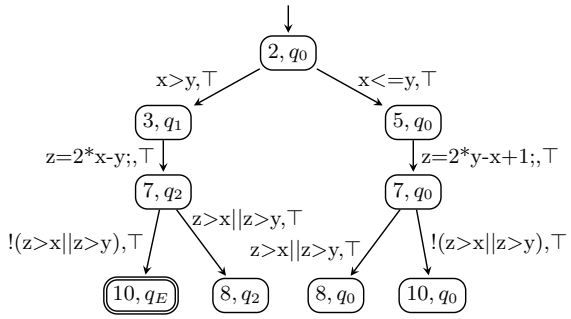

Fig. 5. Product automaton $A_{C \times W_V}$

3.2 Programs from Violation Witnesses

For explaining the validation of results based on a violation witness, we consider the witness in Fig. 4 for our example C program in Fig. 2. The program $C_{C \times W_V}$ resulting from product automaton $A_{C \times W_V}$ in Fig. 5 can be passed to a verifier. If this verification finds an execution that reaches a specification violation, then this violation is guaranteed to be also present in the original program. There is however one caveat: In the example in Fig. 5, a reachable state $(10, q_0)$ at program location 10 (i.e., a state that violates the specification) can be found that is not marked as accepting state in the witness automaton W_V. For a strict version of witness validation, we can remove all states that are in $T \times Q$ but not in $T \times F$ from the product automaton, and thus, from the generated program. This will ensure that if the verifier finds a violation in the generated program, the witness automaton also accepts the found error path. The version of MetaVal that was used in SV-COMP 2020 did not yet support strict witness validation.

3.3 Programs from Correctness Witnesses

Correctness witnesses are represented by observer automata. Figure 6 shows a potential correctness witness W_C for our example program C in Fig. 2, where the invariants are annotated in bold font next to the corresponding state. The construction of the product automaton $A_{C \times W_C}$ in Fig. 7 is a first step towards reestablishing the proof of correctness: the product states tell us to which control locations of the CFA for the program the invariants from the witness belong.

The idea of a result validator for correctness witnesses is to

1. check the invariants in the witness and
2. use the invariants to establish that the original specification holds.

We can achieve the second goal by extracting the invariants from each state in the product automaton $A_{C \times W_C}$ and adding them as conditions to all edges by which the state can be reached. This will then be semantically equivalent to assuming that the invariants hold at the state and potentially make the consecutive proof easier. For soundness we need to also ensure the first goal. To achieve that, we add transitions into a (new) accepting state from $T \times F$ whenever we transition

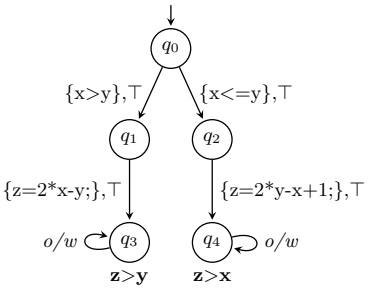

Fig. 6. Correctness witness W_C

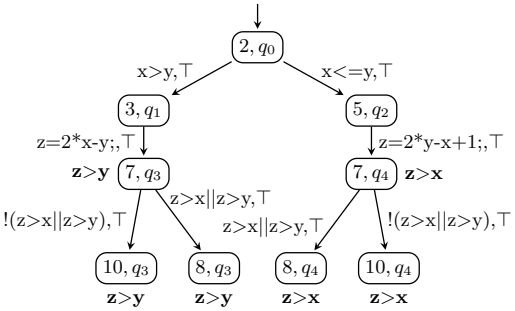

Fig. 7. Product automaton $A_{C \times W_C}$

into a state q and the invariant of q does not hold, and we add self-loops such that the automaton stays in the new accepting state forever. In sum, for each invariant, there are two transitions, one with the invariant as guard (to assume that the invariant holds) and one with the negation of the invariant as guard (to assert that the invariant holds, going to an accepting (error) state if it does not hold). This transformation ensures that the resulting automaton after the transformation is still a proper observer automaton.

4 Evaluation

This section describes the results that were obtained in the 9th Competition on Software Verification (SV-COMP 2020), in which MetaVal participated as validator. We did not perform a separate evaluation because the results of SV-COMP are complete, accurate, and reproducible; all data and tools are publicly available for inspection and replication studies (see data availability in Sect. 6).

4.1 Experimental Setup

Execution Environment. In SV-COMP 2020, the validators were executed in a benchmark environment that makes use of a cluster with 168 machines, each of them having an Intel Xeon E3-1230 v5 CPU with 8 processing units, 33 GB of RAM, and the GNU/Linux operating system Ubuntu 18.04. Each validation run was limited to 2 processing units and 7 GB of RAM, in order to allow up to 4 validation runs to be executed on the same machine at the same time. The time limit for a validation run was set to 15 min for correctness witnesses and to 90 s for violation witnesses. The benchmarking framework BenchExec 2.5.1 was used to ensure that the different runs do not influence each other and that the resource limits are measured and enforced reliably [15]. The exact information to replicate the runs of SV-COMP 2020 can be found in Sect. 3 of the competition report [4].

Benchmark Tasks. The verification tasks[5] of SV-COMP can be partitioned wrt. their specification into ReachSafety, MemSafety, NoOverflows, and Termination. Validators can be configured using different options for each specification.

[5] https://github.com/sosy-lab/sv-benchmarks/tree/svcomp20

Table 1. Overview of validation for violation witnesses in SV-COMP 2020

Specification	Measure	CPAchecker	CPA-wtt	FShell-wtt	MetaVal	nitwit	UAutomizer
ReachSafety (35 652 witnesses)	executed on	35 652	25 812	25 812	35 652	21 636	25 812
	uniquely confirmed	3 043	42	175	44	398	547
	jointly confirmed	8 019	6 010	6 740	1 566	8 055	3 802
Termination (9 720 witnesses)	executed on	3 043			9 720		9 720
	uniquely confirmed	566			9		235
	jointly confirmed	1 539			256		1 493
NoOverflow (3 149 witnesses)	executed on	3 149	3 149	3 149	3 149		3 149
	uniquely confirmed	6	1	31	1		89
	jointly confirmed	1 668	1 067	1 267	1 186		1 590
MemSafety (2 681 witnesses)	executed on	2 681	2 213	2 681	2 681		2 681
	uniquely confirmed	278	0	21	113		44
	jointly confirmed	737	250	364	478		372

Table 2. Overview of validation for correctness witnesses in SV-COMP 2020

Specification	Measure	CPAchecker	MetaVal	UAutomizer
ReachSafety (66 435 witnesses)	executed on	66 435	66 435	66 435
	uniquely confirmed	1 750	391	708
	jointly confirmed	17 592	13 862	16 834
NoOverflow (3 179 witnesses)	executed on		3 179	3 179
	uniquely confirmed		44	74
	jointly confirmed		870	870
MemSafety (4 426 witnesses)	executed on		4 426	4 426
	uniquely confirmed		398	173
	jointly confirmed		811	811

Validator Configuration. Since our architecture (cf. Fig. 1) allows for a wide range of verifiers to be used for validation, there are many interesting configurations for constructing a validator. Exploring all of these in order to find the best configuration, however, would require significant computational resources, and also be susceptible to over-fitting. Instead, we chose a heuristic based on the results of the competition from the previous year, i.e., SV-COMP 2019 [3]. The idea is that a verifier which performed well at *verifying* tasks for a specific specification is also a promising candidate to be used in *validating* results for that specification. Therefore the configuration of our validator MetaVal uses CPA-Seq as verifier for tasks with specification ReachSafety, Ultimate Automizer for NoOverflow and Termination, and Symbiotic for MemSafety.

4.2 Results

The results of the validation phase in SV-COMP 2020 [5] are summarized in Table 1 (for violation witnesses) and Table 2 (for correctness witnesses). For each specification, MetaVal was able to not only confirm a large number of results

that were also validated by other tools, but also to confirm results that were not previously validated by any of the other tools.[6]

For violation witnesses, we can observe that MetaVal confirms significantly less witnesses than the other validators. This can be explained partially by the restrictive time limit of 90 s. Our approach not only adds overhead when generating the program from the witness, but this new program can also be harder to parse and analyze for the verifier we use in the backend. It is also the case that the verifiers that we use in MetaVal are not tuned for such a short time limit, as a verifier in the competition will always get the full 15 min. For specification ReachSafety, for example, we use CPA-Seq, which starts with a very simply analysis and switches verification strategies after a fixed time that happens to be also 90 s. So in this case we will never benefit from the more sophisticated strategies that CPA-Seq offers.

For validation of correctness witnesses, where the time limit is higher, this effect is less noticeable such that the number of results confirmed by MetaVal is more in line with the numbers achieved by the other validators. For specification MemSafety, MetaVal even confirms more correctness witnesses than Ultimate Automizer. This indicates that Symbiotic was a good choice in our configuration for that specification. Symbiotic generally performs much better in verification of MemSafety tasks than Ultimate Automizer, so this result was expected.

Before the introduction of MetaVal, there was only one validator for correctness witnesses in the categories NoOverflow and MemSafety, while constructing a validator for those categories with our approach did not require any additional development effort.

5 Related Work

Programs from Proofs. Our approach for generating programs can be seen as a variant of the Programs from Proofs (PfP) framework [27,41]. Both generate programs from an abstract reachability graph of the original program. The difference is that PfP tries to remove all specification violations from the graph, while we just encode them into the generated program as violation of the standard reachability property. We do this for the original specification and the invariants in the witness, which we treat as additional specifications.

Automata-Based Software Model Checking. Our approach is also similar to that of the validator Ultimate Automizer [10]. For violation witnesses, it also constructs the product of CFA and witness. For correctness witnesses, it instruments the invariants directly into the CFA of the program (see [10], Sect. 4.2) and passes the result to its verification engine, while MetaVal constructs the product of CFA and witness, and applies a similar instrumentation. In both cases, MetaVal's transformer produces a C program, which can be passed to an independent verifier.

Reducer-Based Conditional Model Checking. The concept of generating programs from an ARG has also been used to successfully construct conditional verifiers [14].

[6] In the statistics, a witness is only counted as confirmed if the verifier correctly stated whether the input program satisfies the respective specification.

Our approach for correctness witnesses can be seen as a special case of this technique, where MetaVal acts as initial verifier that does not try to reduce the search space and instead just instruments the invariants from the correctness witness as additional specification into the program.

Verification Artifacts and Interfacing. The problem that verification results are not treated well enough by the developers of verification tools is known [1] and there are also other works that address the same problem, for example, the work on execution reports [19] or on cooperative verification [17].

Test-Case Generation. The idea to generate test cases from verification counterexamples is more than ten years old [8,39], has since been used to create debuggable executables [31,33], and was extended and combined to various successful automatic test-case generation approaches [24,25,29,35].

Execution. Other approaches [18,22,28] focus on creating tests from concrete and tool-specific counterexamples. In contrast, witness validation does not require full counterexamples, but works on more flexible, possibly abstract, violation witnesses from a wide range of verification tools.

Debugging and Visualization. Besides executing a test, it is important to understand the cause of the error path [23], and there are tools and methods to debug and visualize program paths [2,9,26].

6 Conclusion

We address the problem of constructing a tool for witness validation in a systematic and generic way: We developed the concept of *validation via verification*, which is a two-step approach that first applies a program transformation and then applies an off-the-shelf verification tool, without development effort.

The concept is implemented in the witness validator MetaVal, which has already been successfully used in SV-COMP 2020. The validation results are impressive: the new validator enriches the competition's validation capabilities by 164 uniquely confirmed violation results and 834 uniquely confirmed correctness results, based on the witnesses provided by the verifiers. This paper does not contain an own evaluation, but refers to results from the recent competition in the field.

The major benefit of our concept is that it is now possible to configure a spectrum of validators with different strengths, based on different verification engines. The 'time to market' of new verification technology into validators is negligibly small because there is no development effort necessary to construct new validators from new verifiers. A potential technology bias is also reduced.

Data Availability Statement. All data from SV-COMP 2020 are publicly available: witnesses [7], verification and validation results as well as log files [5], and benchmark programs and specifications [6][7]. The validation statistics in Tables 1 and 2 are available in the archive [5] and on the SV-COMP website[8]. MetaVal 1.0 is available on GitLab[9] and in our AEC-approved virtual machine [16].

[7] https://github.com/sosy-lab/sv-benchmarks/tree/svcomp20
[8] https://sv-comp.sosy-lab.org/2020/results/results-verified/validatorStatistics.html
[9] https://gitlab.com/sosy-lab/software/metaval/-/tree/1.0

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Recursive Data Structures in SPARK

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Abstract. SPARK is both a deductive verification tool for the Ada language and the subset of Ada on which it operates. In this paper, we present a recent extension of the SPARK language and toolset to support pointers. This extension is based on an ownership policy inspired by Rust to enforce non-aliasing through a move semantics of assignment. In particular, we consider pointer-based recursive data structures, and discuss how they are supported in SPARK. We explain how iteration over these structures can be handled using a restricted form of aliasing called local borrowing. To avoid introducing a memory model and to stay in the first-order logic background of SPARK, the relation between the iterator and the underlying structure is encoded as a predicate which is maintained throughout the program control flow. Special first-order contracts, called pledges, can be used to describe this relation. Finally, we give examples of programs that can be verified using this framework.

Keywords: Deductive verification · Recursive structures · Ownership

1 Introduction

The programming language SPARK [8] has been designed to be amenable to formal verification, and one of the most impactful design choices was the exclusion of aliasing. While this choice vastly simplified the tool design and improved the expected proof performance, it also meant that pointers, as a major source of aliasing, were excluded from the language. While SPARK over the years had seen the addition of many language features, adding pointers just seemed impossible without violating the non-aliasing property. Then came Rust [11] democratizing a type system based on ownership [5]. Taking inspiration from it, it was possible to add pointers to the language in a way that still excludes aliasing. We will give an overview of the rules in this paper.

However, it was unclear if programs traversing recursive data structures such as lists and trees could be supported in this setting. In particular, iteration using a loop requires an alias between the traversed structure and the iterator. In this paper, we detail an approach, inspired by recent work by Astrauskas et al. [1], that enables proofs about recursive pointer-based data structures in SPARK. We have implemented this approach in the industrial formal verification tool SPARK, and, using this tool, developed a number of examples. Some important restrictions remain - we will also discuss them in this paper.

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Ada [2] is a general-purpose procedural programming language. The design of the Ada language puts great emphasis on the safety and correctness of the program. This objective is realized by using a readable syntax that uses keywords instead of symbols where reasonable. The type system is strong and strict and many potential violations of type constraints can be detected statically by the compiler. If not, a run-time check is inserted into the program, to guarantee the detection of incorrect situations.

```
declare              --  Block introducing new declarations
  type My_Int is range -100 .. 100;
  -- User-defined integer type ranging from -100 to 100
  subtype My_Nat is My_Int range 0 .. My_Int'Last;
  -- Subtype of My_Int with additional constraints

  X : My_Int := 50; --  Static check that 50 is in the bounds of My_Int
  Y : My_Nat;
begin                --  Part of the block containing statements
  ...
  Y := X;            --  Dynamic check that X is in the bounds of My_Nat
end;                 --  End of scope of the entities declared in the block
```

Ada 2012 introduced contract based programming to Ada. In particular, it is possible to attach pre- and postconditions to subprograms[1]. These conditions can be checked during the execution of the program, just like assertions.

SPARK is the name of a tool that provides formal verification for Ada. It uses the user-provided contracts and attempts to prove that the runtime checks cannot fail and that postconditions are established by the corresponding subprograms. As formal verification for the whole Ada language would be intractable, SPARK is also the name of the subset of the Ada language that is supported by the SPARK tool[2]. This subset contains almost all features of Ada, though sometimes in a restricted form. In particular, expressions should be free from side effects, and aliasing is forbidden (no two variables should share the same memory location or overlap in memory). This restriction greatly simplifies the memory model used in the SPARK tool: any program variables can be reasoned about independently from other variables.

The SPARK tool uses the Why3 platform to generate verification conditions for SMT solvers via a weakest-precondition calculus [4].

2 Support for Pointers

Pointers in Ada are called *access types*. It is possible to declare an access type using the `access` keyword. Objects of an access type are `null` if no initial values are supplied. It is possible to allocate an object on the heap using the keyword `new`. An initial value can be supplied for the allocated object. A dereference of a pointer is written as a record component access, but using the keyword `all`.

[1] In Ada, a distinction is made between functions that return a value, and procedures, which do not. *Subprogram* is the term that designates both.

[2] http://docs.adacore.com/spark2014-docs/html/ug/.

```
declare
  type Int_Acc is access Integer; --  Declare a new access type
  X : Int_Acc;                    --  Declare an object of this type
  pragma Assert (X = null);       --  No initial values provided, X is null
  Y : Integer;
begin
  X := new Integer;             --  Allocation of uninitialized data
  X := new Integer'(3);         --  Allocation of initialized data
  Y := X.all;                   --  Dereference the access
end;
```

When a pointer is dereferenced, a runtime check is introduced to make sure that it is not null. Ada does not mandate garbage collection. Memory allocated on the heap can be reclaimed manually by the user using a generic function named `Unchecked_Deallocation`, which also sets its argument pointer to null. There are several kinds of access types. The basic access types, like `Int_Acc` defined above, are called pool specific access types. They can only designate objects allocated on the heap. General access types, introduced by the keyword `all`, can also be used to designate objects allocated on the stack or global data.

Pointers were excluded from the SPARK subset until recently. Indeed, allowing pointers in a straightforward way would break the absence of aliasing in SPARK. In addition, pointers are associated with a list of classes of bugs such as memory leaks, use-after-free and dereferencing a null-pointer.

To support pointers in SPARK, we designed a subset of Ada's access types which does not introduce aliasing and avoids some pointer-specific issues, while retaining as much expressivity as possible. The first restriction we selected is the exclusion of general access types. This means that SPARK can only create pointers designating memory allocated on the heap, and not on the stack. As a result, pointers can only be made invalid by explicit deallocation, and deallocation of a valid pointer is always legal. To eliminate aliasing between (heap) pointers, ownership rules inspired by Rust have been added on top of Ada's legality rules. These rules enforce a single writer/multiple readers policy. They ensure that, when a value designated by a pointer is modified, all other objects can be considered to be preserved.

The basis of the ownership policy of SPARK is the move semantics of assignments. When a pointer is assigned to a variable, both the source and the target of the assignment designate the same memory region: assigning an object containing a pointer creates an alias. To alleviate this problem, when an object containing a pointer is assigned, the memory region designated by the pointer is said to be *moved*. The source of the assignment loses the ownership of the designated data while the target of the assignment gains it. The ownership system makes sure that the designated data is not accessed again through the source of the assignment.

```
Y : Int_Acc := X;   -- Ownership of the data designated by X is moved to Y
Y.all := Y.all + 1; -- The data can be read and modified through Y
Z := X.all;         -- Illegal: Reading or modifying X.all is not allowed
```

As the ownership policy ensures that no aliasing can occur between access objects, it is possible to reason about the program almost as if the pointer was replaced by the data it points to. When an object containing a pointer is

assigned to another variable, it is safe to consider that the designated data is copied by the assignment. Indeed, any effects that could occur because variables are sharing a substructure cannot be observed because of the ownership rules.

Pointers are handled in the verification model of the SPARK proof tool as *maybe*, or *option* types: access objects are either null, or they contain a value. In addition, access objects also contain an address, which can be used to handle comparison (two pointers may not be equal even if the values they designate are equal). When a pointer is dereferenced, a verification condition is generated to make sure that the pointer is not null, so that its value can be accessed.

```
X : Int_Acc;           --  X is null
X := new Integer'(3); --  X has a value which is 3
Y := X;                --  Y has a value which is 3
Z := Y.all;            --  Check that Y is not null, Z is 3
```

Note that the ownership policy is key for this translation to be correct, as it prevents the program from observing side-effects caused by the modification of a shared reference, which would not be accounted for in the verification model.

3 Recursive Data Structures

In Ada, recursivity can only be introduced through pointers. The idea is to first declare a type, but without giving its definition. This declaration, called an *incomplete declaration*, introduces a place-holder for the type, which can only be used in restricted circumstances. In particular, this place-holder can be used to declare an access type designating pointers to values of this type. Using this mechanism, it is possible to declare a recursive data structure, since the access type can be used in the type definition as it comes afterward.

```
type List_Cell;
type List is access List_Cell;
type List_Cell is record
  Data : Integer;
  Next : List;
end record;
```

There are no specific restrictions concerning recursive types in SPARK. However, the ownership policy of SPARK implies that it will not be possible to create a structure which has either cycles (e.g. doubly linked lists) or shared substructures (e.g. DAGs) in it. The ownership policy may also impact how recursive structures can be manipulated. In general, working with such structures involves a traversal, which can be done either recursively, or iteratively using a loop. Algorithms working in a recursive way are generally compliant with the ownership policy of SPARK. Indeed, the recursive calls will allow reading or modifying the structure in depth without having to deconstruct it[3].

```
function Length (L : access constant List_Cell) return My_Nat is
  (if L = null then 0 else Length (L.Next) + 1);
function Nth (L : access constant List_Cell; N : My_Pos) return Integer is
  (if N = 1 then L.Data else Nth (L.Next, N - 1))
with Pre ⇒ N ≤ Length (L);
```

[3] In `Length` and `Nth`, addition on `My_Nat` and `My_Pos` has been redefined to saturate so as to avoid the overflow checking mandated by Ada.

Algorithms involving loops are trickier. The declaration of the iterator used for the loop creates an alias of the traversed data structure. As per SPARK's ownership policy, this is considered to be a move, so it makes it illegal to access the initial structure. Further assignments to the iterator during the traversal contribute to losing definitively one by one the ownership of every node in the structure, making it impossible to restore the ownership at the end.

```
procedure Set_All_To_Zero (X : in out List) is
   Y : List := X;    -- The ownership of X is transferred to Y
begin
   while Y ≠ null loop
      Y.Data := 0;
      Y := Y.Next;   --  Ownership of the first cell of Y is lost for good
   end loop;         --  The ownership of X cannot be restored
end Set_All_To_Zero;
```

To traverse recursive data structures, a move is not what we want. Here we need a way to lend the ownership of a memory region for a period of time and automatically restore it at the end. A similar mechanism, called *borrowing*, is available in the Rust language. We have adapted it to SPARK.

4 Borrowing Ownership

As Ada is an imperative language, losing the possibility to traverse a linked data structure using a loop was deemed too restrictive. To alleviate this problem, a notion of ownership borrowing was introduced in SPARK. It allows the users to declare a variable, called a borrower, which is initialized with a reference to a part of an existing data structure. To state that this initialization should not be considered a move, an *anonymous access type* is used for the borrower[4]. During the scope of the borrower, the borrowed part of the underlying structure is frozen, meaning that it is illegal to read or modify it. Once the borrower has gone out of scope, the ownership automatically returns to the borrowed object, so that it is again fully accessible.

```
X := ...;                       --  X is initialized to the list {1,2,3,4}
declare
  Y : access List_Cell := X;    --  Y has an anonymous access type.
  --  Ownership of X is transferred to Y for the duration of its lifetime.
begin
  Y.Data := Y.Data + 1;         --  Y can be used to read or modify X
  pragma Assert (X.Data = 2);   --  Illegal, during the lifetime of Y, X
                                --  cannot be read or modified directly
end;
pragma Assert (X.Data = 2);     --  Afterwards, the ownership returns to X
```

A borrower can be used to modify the underlying structure. This makes it effectively an alias of the borrowed object. To allow the tool to statically determine the cases of aliasing, SPARK restricts the initial value of a local borrower to be the name of a part of an existing object. This forbids for example borrowing one of two structures depending on a condition.

[4] A type is said to be anonymous if it does not have a previous declaration. Here `access List_Cell` is anonymous while `List` is named.

It is possible to update a borrower to change the part of the object it designates (as opposed to modifying the designated object). This is called a reborrow. In SPARK, the value assigned to the borrower in a reborrow should be rooted at the borrower. This means that reborrows only go deeper into the structure.

```
declare
  Y : access List_Cell := X;  --  Y is X
begin
  Y := Y.Next;                --  This is a reborrow, Y is now X.Next
end;
```

Borrowing can be used to allow simple iterative traversals of a recursive data structure like the loop of `Set_All_To_Zero`. More complex traversals, involving stacks for example, cannot be written iteratively in SPARK.

```
procedure Set_All_To_Zero (X : in out List) is
   Y : access List_Cell := X;
   -- The ownership of X is transferred to Y for the duration of its lifetime
begin
   while Y ≠ null loop
      Y.Data := 0;
      Y := Y.Next;   --  Reborrow: Y designates something deeper
   end loop;
end Set_All_To_Zero; --  The ownership of X is restored
```

Using reborrows, local borrowers allow one to indirectly modify a data structure at an arbitrarily-deep position, which may not be statically-known. While in the scope of the borrower, these indirect modifications can be ignored by the analysis, as the ownership policy makes them impossible to observe. However, after the end of the borrow, ownership is transferred back to the borrowed object, and SPARK needs to take into account whatever modifications may have occurred through the borrower.

```
X := ...; --  X is initialized to the list {1,2,3,4}
declare
  Y : access List_Cell := X;            --  Y is X
begin
  Y := Y.Next.Next;
  --  Through reborrows, Y designates an arbitrarily-deep part of X
  Y.Data := 42;                         --  Y is used to indirectly modify X
end;
pragma Assert (X.Next.Next.Data = 42);  --  The assertion should hold
```

To be able to reconstruct the borrowed object from the value of the borrower, we must track the relation between them. As this relation cannot be statically determined because of reborrows, SPARK handles it as an additional object in the program. This allows us to take advantage of the normal mechanism for handling value dependent control-flow in SPARK (the weakest-precondition calculus of Why3). The idea is the following. When a borrower is declared in Ada, we create two objects: the borrower itself, which is considered as a stand-alone structure, independent of the borrowed object, and a predicate. The predicate, which we call the borrow relation, encodes the most precise relation between the borrower and the borrowed object which does not depend on the actual value designated by the borrower. The value of the *borrow relation* is computed by the tool from the definition of the borrower, and is updated at each reborrow. Modifications of the underlying data structure don't impact this relation. At the

end of the borrow, the borrowed object is reconstructed using both the borrow relation and the current value of the borrower.

```
X := ...; --  X is initialized to the list {1,2,3,4}
declare
  Y : access List_Cell := X; --  Create borrow relation to relate X and Y
  --  b_rel := λ new_x, new_y. new_x ≠ null ∧ new_x = new_y
begin
  Y := Y.Next.Next; --  Update the predicate to model the new relation
  --  b_rel := λ new_x, new_y. new_x ≠ null ∧ new_x.data = 1 ∧
  --    new_x.next ≠ null ∧ new_x.next.data = 2 ∧ new_x.next.next ≠ null
  --    ∧ new_x.next.next = new_y
  Y.Data := 42; --  The borrow relation is not modified
end;
pragma Assert (X.Next.Next.Data = 42);
--  Follows from the fact that X.Next.Next = Y and Y.Data = 42
```

5 Describing the Borrow Relation

SPARK performs deductive verification, which relies on user-specified invariants to handle loops. When traversing a linked data structure, the loop body contains a reborrow, which means that the borrow relation is modified in the loop. As a general rule, if a variable is modified in a loop, it should be described in the loop invariant, lest nothing is known about its value afterward. Thus, we need a way to describe the borrow relation in the loop invariant.

As part of their work on the Prusti proof tool for Rust, Astrauskas et al. found the need for a similar annotation that they call *pledges* [1]. In Rust, a pledge is an assertion associated with a borrower which is guaranteed to hold at the time when the borrow expires, no matter what may happen in between. In SPARK, a property guaranteed to hold at the end of the borrow must be a consequence of the borrow relation, since the borrow relation is the most precise relation which does not depend on the actual value of the borrower. Therefore, the user-visible notion of a pledge is suitable to approximate the internally computed borrow relation. Similar to user-provided postconditions, which must be implied by the strongest postcondition computed by a verifying tool, the user-provided pledge should follow from the borrow relation.

Since the Ada syntax has no support for pledges, we have resorted in SPARK to introducing special functions (dedicated to each access type) called pledge functions, which mark expressions which should be considered as pledge expressions by the tool. A pledge function is a *ghost* function (meaning that it is not allowed to have any effect on the output of the program) which has two parameters. The first one is used to identify the borrower on which the pledge should apply, while the second holds the assertion. Note that a call to a pledge function isn't really a call for the SPARK analyzer. It is simply a marker that the expression in argument is a pledge.

```
function Pledge
  (L : access constant Cell; --  The borrower to which the pledge applies
   P : Boolean)              --  The property we want to assert in the pledge
    return Boolean
is (P)  --  For execution, the function evaluates the property
with Ghost,
  Annotate ⇒ (GNATprove, Pledge); --  Identifies a pledge function for SPARK
```

When a pledge function is called in an assertion, SPARK recognizes it and identifies its parameter as a pledge. It therefore attempts to show that the property is implied by the borrow relation (as opposed to implied by the current value of the borrower).

```
X := ...; --  X is initialized to the list {1,2,3,4}
declare
  Y : access List_Cell := X;
begin
  Y := Y.Next.Next;
  pragma Assert (Pledge (Y, Y = X.Next.Next));
  --  True as this is implied by borrow relation
  pragma Assert (Pledge (Y, X.Data = 1 and X.Next.Data = 2));
  --  True again as the first 2 elements of X are frozen
  pragma Assert (Pledge (Y, X.Next.Next.Data = 3));
  --  False, though this is true at the current program point, as it is not
  --  guaranteed to hold at the end of the borrow.
  ...
end;
```

Using pledges, we can formally verify the `Set_All_To_Zero` procedure. Its postcondition states that all elements of the list have been set to 0 using the Nth function. To be able to express the loop invariant in a similar way, we have introduced a ghost variable C to count the number of iterations. Its value is maintained by the first loop invariant. The second and third invariants are pledges, describing how the value of X can be reconstructed from the value of the iterator Y. The second invariant gives the length of the list, while the third describes the value of its elements using the Nth function. Elements which have already been processed are frozen by the borrow. Their value is known to be 0. Other elements can be linked to the corresponding position in the iterator Y.

```
procedure Set_All_To_Zero (X : List) with
  Pre  ⇒ Length (X) < My_Nat'Last,
  Post ⇒ Length (X) = Length (X)'Old
    and (for all I in 1 .. Length (X) ⇒ Nth (X, I) = 0);
  --  All elements of X are 0 after the call

procedure Set_All_To_Zero (X : List) is
   C : My_Nat := 0 with Ghost;
   Y : access List_Cell := X;
begin
   while Y ≠ null loop
      pragma Loop_Invariant (C = Length (Y)'Loop_Entry - Length (Y));
      --  C elements have been traversed
      pragma Loop_Invariant
        (Pledge (Y, Length (X) = Length (Y) + C));
      pragma Loop_Invariant
        (Pledge (Y, (for all I in 1 .. Length (X) ⇒
           Nth (X, I) = (if I ≤ C then 0 else Nth (Y, I - C)))));
      --  All elements are 0 up to C, others are elements of Y
      Y.Data := 0;
      Y := Y.Next;
      C := C + 1;
   end loop;
end Set_All_To_Zero;
```

Note that, in general, it is not necessary to write a pledge to verify a program using a local borrower. Indeed, the analysis tool is able to precisely track the borrow relation through successive reborrows. Pledges need only be provided when the borrow relation itself cannot be tracked by the tool, for example because of a loop, like in our example.

6 Evaluation

We could not try the tool on any pre-existing benchmark since SPARK codebases do not have pointers, and Ada codebases usually violate some SPARK rules. In particular, Ada codebases have no reason to abide by the ownership policy of SPARK. So instead, we mostly had to write new tests to assess the correctness and performance of our implementation. The public testsuite of SPARK contains more than 150 tests mentioning access types, be they supported cases or not.

To assess expressivity and provability on programs dealing with recursive data structures, we have written 6 examples, none of them very big, but ranging over various levels of complexity[5]. On all of these examples, we have shown that the runtime checks imposed by the Ada language are guaranteed to pass and that no uninitialized value can be read. In addition, we have manually supplied functional properties.

Figure 1 gives some metrics over these examples. Under the tab Loc are listed the total number of lines of code in the example, the number of lines of specification (including contracts and specification functions), and the number of additional ghost annotations (assertions, loop invariants, ghost variables...). The #Checks column gives the number of checks generated by the tool (contracts, assertions, invariants, language defined checks...). In the last three columns, we can see the total running time of SPARK, both from scratch using its default strategy and only replaying the proofs through the replay facility, as well as the maximal time needed to prove a single verification condition.

Example	#Subp	LOC			#Checks	Analysis time (s)		
		All	Spec	Ghost		Default	Replay	Max VC
set all to zero	5	57	19 (33%)	8 (14%)	25	4	3	< 1
linear search	7	136	67 (49%)	24 (17%)	109	10	9	< 1
pointer-based maps	7	130	38 (29%)	12 (9%)	64	6	5	< 1
route shift	8	99	50 (50%)	3 (3%)	64	9	6	< 1
binary search	13	239	99 (41%)	42 (17%)	129	24	17	4
red black trees	37	611	107 (17%)	384 (63%)	920	258	152	16

Fig. 1. Overview of the examples involving recursive data structures

Though these examples are small, we think they demonstrate that it is possible to define recursive data structures in SPARK, and to verify iterative programs using them. When writing the algorithms, we found that the limitations mostly come from the ownership policy of SPARK. Some data structures are not supported, requiring either to switch to full Ada for their implementations, or to change the algorithm to work around the missing links. In general, we found

[5] https://github.com/AdaCore/spark2014/tree/master/papers/Pledge2020/examples.

that the annotation effort required to describe the borrow relations, though non-negligible, was acceptable. In particular, it uses the standard SPARK expressions, with no mentions of memory separation or permission.

7 Related Work

Program verification tools for mainstream languages such as C or Java generally support aliasing, because the concept of pointer or reference is more central. They deal with it by modeling the heap. The WP plugin of Frama-C uses by default a *typed memory model* where different arrays are used for the basic types of C [6]. The VerCors [3] toolset handles high-level programming languages, such as Java, by extending the annotation language with separation logic with permission [10]. In SPARK we have chosen a different approach, as we avoid modeling the heap completely by using ownership rules to enforce non-aliasing.

The ownership rules introduced in SPARK are largely inspired by the Rust language [11]. The differences are mostly motivated by the need to comply with the preexisting Ada semantics of pointers. In addition, SPARK was aiming at coming up with a subset as easy to verify as possible. The resulting model is simpler because it does not make lifetime of borrowers explicit, and aliases created through borrows are always statically known.

The Prusti verification tool for Rust [1] allows users to verify that a program complies with its specification. Both tools provide similar guarantees and require similar annotations. However, they differ in their implementation. Indeed, Prusti works by translating separation constraints enforced by the Rust type system to the intermediate verification language of the Viper tool [9]. Our work differs here, as we use the ownership system to abstract away memory related concerns, so that the verification process does not need to be aware of them.

In a recent work [7], Matsushita et al. propose a translation to CHCs for Rust programs. Like in our approach, the restrictions imposed by the ownership policy are key for the soundness of their method. However, while we introduce the notion of borrow relation to be able to use a standard WP calculus, they present a new calculus specifically tailored to Rust references.

8 Conclusion

We have presented a recent extension of the SPARK language and toolset to support pointers. It is based on an ownership policy enforcing non-aliasing. To support pointer-based recursive data structures, a restricted form of aliasing is introduced in SPARK through local borrowers, which can be used to iterate through a linked data structure in an imperative way. We have described how local borrowers can be supported by the verification tool, without introducing a memory model, by using a mutable predicate named the borrow relation. This borrow relation can be described when necessary using special annotations named pledges, which solely consist of SPARK standard expressions, and do not

expose the underlying verification technique. Our work is available in the 20.1 release of SPARK Pro and will be part of the next community release.

As for future work, we would like to extend the subset of Ada pointers supported in SPARK. In particular, we would like to introduce function pointers to model callbacks, pointers to constants with a more permissive ownership policy, and local borrowing of objects allocated on the stack.

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Ivy: A Multi-modal Verification Tool for Distributed Algorithms

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Abstract. Ivy is a multi-modal verification tool for correct design and implementation of distributed protocols and algorithms, supporting modular specification, implementation and proof. Ivy supports proving safety and liveness properties of parameterized and infinite-state systems via three modes: deductive verification using an SMT solver, abstraction and model checking, and manual proofs using natural deduction. It supports light-weight formal methods via compositional specification-based testing and bounded model checking. Ivy can extract executable distributed programs by translation to efficient C++ code. It is designed to support decidable automated reasoning, to improve proof stability and to provide transparency in the case of proof failures. For this purpose, it presents concrete finite counterexamples, automatically audits proofs for decidability of verification conditions, and provides modular hiding of theories.

1 Introduction

Ivy is an open-source [16] multi-modal verification tool for correct design and implementation of distributed algorithms, supporting modular specification, implementation and proof. The motivating principles of Ivy are *predictability*, *stability* and *transparency*. That is, automated proof steps should provide complexity bounds, should be insensitive to small perturbations, and when they fail should provide actionable feedback. To the extent consistent with these principles, Ivy aims to maximize expressiveness and proof automation, and thus to achieve a high level of user productivity in designing, implementing and proving programs. A major goal of Ivy is to support *decidable reasoning*. That is, automated proof should be restricted to logical fragments for which the tool is a decision procedure. This greatly improves the stability of automated provers, which otherwise rely on fragile heuristics to avoid divergence [28]. This is important for the maintenance of large proofs, to prevent small changes from creating unpredictable proof failures. Moreover, on decidable problems, provers fail transparently by providing true counterexamples, which greatly simplifies the iterative development of proofs. Ivy supports the decomposition of proofs to decidable theories by the use of modular abstraction.

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The architecture of Ivy is depicted in Fig. 1. The figure shows the major components of the tool and the information flow between them. Ivy provides a language (also called "Ivy") for the modular description of distributed programs, along with their specifications and proofs (see Sect. 2). Ivy is a synchronous, reactive programming language [3], meaning that the program only executes actions in response to input from its environment, and these actions appear to execute atomically. From an Ivy program, the tool can extract an asynchronous, distributed implementation. A program is made up of reactive modules [1], each having a temporal assume/guarantee-style specification. After parsing of this description and elaboration of templates, the program is decomposed into its component modules, each with associated assumptions and proof obligations, according to a system of proof rules for circular assume/guarantee reasoning (see Sect. 2.1).

These proof obligations are passed on to the tactics engine (see Sect. 3). This engine orchestrates the use of various built-in proof tactics, including decidable invariant checking with an SMT solver (Sect. 3.1), model checking with eager abstraction [19] (Sect. 3.2), liveness proof by translation to safety (Sect. 3.3) and logical deduction rules (Sect. 3.4). Each tactic works by reducing a given proof goal to a (possibly empty) set of sub-goals, from which the original goal can be proved. Combined with modular reasoning, the tactics engine makes it possible to use a variety of proof approaches and proof automation tools in constructing a proof.

Ivy extracts executable distributed programs by translation to C++ (see Sect. 5). From the specifications of a module, Ivy can also generate a modular randomized specification-based tester [7] (see Sect. 4.1). This also makes it possible to test infrastructure not written in Ivy (including hardware) against Ivy specifications.

1.1 Related Work

Ivy can be thought of as a hybrid between program verification tools such as ESC-Java [11] and Dafny [14], based on the Floyd/Hoare approach, compositional model checking tools, such as Mocha [2] and Cadence SMV [17] and proof assistants based on the LCF model, such as Isabelle [26] or Coq [4]. Compared to program verification tools that support only procedure modularity, Ivy provides a richer form of specification that allows complete hiding of internal state, and provides architectural support for decidable reasoning (see Sect. 2.1). Compared to compositional tools, Ivy integrates a richer variety of reasoning techniques (see Sect. 3). Compared to proof assistants, Ivy provides domain-specific support for decidable proof automation, supporting a greater degree of proof automation [28]. On the other hand, Ivy relies on a vastly larger trusted computing base than typical proof assistants. Moreover, Ivy has no mechanism of reflection, and thus cannot be used for meta-reasoning about programs and program transformations. In principle, all the techniques in Ivy could be integrated into a tool such as Isabelle or Coq but the effort would be large. A less foundational tool such as

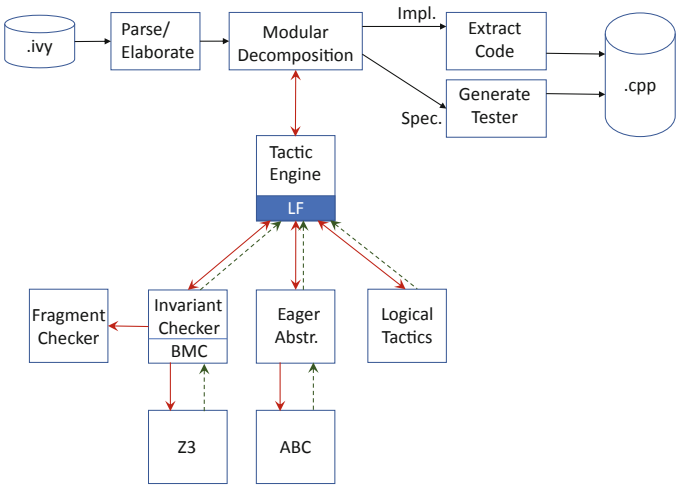

Fig. 1. Ivy architecture, showing flow between major components. Red, solid arrows represent flow of proof goals and assumptions. Green, dashed arrows represent flow of proofs and/or counterexamples. Not shown is VC generator, shared between Invariant Checking/BMC and Eager Abstraction components. (Color figure online)

Ivy makes it possible to rapidly experiment with new proof and proof automation strategies. Compared to all of these tools, Ivy differs in providing native support for extracting distributed programs, and specification-based testing. A related tool, mypyvy, focuses on more powerful invariant inference techniques, but lacks the other features of Ivy [10,29].

2 A Modular Language for Decidable Reasoning

The primary design goal of Ivy's language is to support decidable reasoning while maximizing expressiveness and performance. Figure 2 is an example of the basic unit of verification in Ivy, called an *isolate*. An isolate is a reactive module that hides internal state and provides a temporal (that is, stateful) specification of its interface. An isolate has named traits that include types, properties, variables and actions. It is divided into a *specification* part and an *implementation* part. The figure shows an example of a simple module that inputs a sequence of numbers and outputs an upper bound on the numbers received thus far.

Types, Variables and Actions. The native datatypes in Ivy include just the Boolean type, uninterpreted types, records (structs) over datatypes, and pure first-order functions. In the figure, line 2 declares an uninterpreted type t. Line 6 declares a state variable 'seen' holding a predicate over t. This variable is initialized at line 9. This assigns 'seen(X)' to be the function that returns false for all values of X.

Procedures in Ivy are called *actions* and may have side effects on variables. Parameters are passed by value and there are no references. This greatly simplifies modular reasoning (see Sect. 2.1) and also allows for aggressive compiler optimizations due to the absence of aliasing (see Sect. 5).

In the figure, line 3 declares an action 'ub' that takes an input x of type t and outputs y of type t. Its implementation is given at lines 24 to 27. It updates a state variable 'max' holding the maximum value received thus far, and returns this value by assigning it to the output variable y.

2.1 Modularity and Decidability

The specification part of the isolate (lines 5 to 18) consists of *ghost* variables and code that are *visible* outside the isolate. The implementation part (lines 19 to 30) consists of *real* variables and code that are *invisible* outside the module. At line 15 the ghost predicate 'seen' is updated to reflect the fact that value x has been seen as an input. Specification code contains assume/guarantee specifications in terms of `require` and `ensure` statements. For example, line 12 represents an assumption that input values are non-negative. Line 16 represents a guarantee that output values will be an upper bound on all seen values.

Ghost and real code are kept syntactically separate in Ivy. The specification code is interleaved with the implementation code using the directives 'before' (line 11) and 'after' (line 14). Thus, in the figure, the 'require' statement acts as a precondition, while the 'ensure' statement acts as a postcondition. The implementation code is not allowed to side effect any externally visible state, so it is sound to erase (or 'slice') this code when verifying other modules. Other modules see only the ghost code, which provides an abstract model of the isolate. Similarly, when extracting executable code, it is safe to erase the ghost code (which must be proven to be terminating). This makes it possible, for example, to provide a pure, functional specification of a module interface, even though internally it has state.

Theories can also be hidden inside modules. For example, the implementation of our example interprets the type t as the integers (line 28). For verification purposes, this instantiates the theory of Peano arithmetic for type t. This theory is used *only* to prove correctness of the isolate, and is invisible to other isolates. The theory can be used to prove properties (such as the irreflexivity property at line 7) that provide an abstraction of the type externally. The ability to hide theories behind abstractions provides an important strategy for keeping proof obligations decidable.

An isolate with no implementation part (that is, a "ghost" module) can act as an abstract model of a protocol. Using Ivy's modular rules, an abstract model can be *refined* to an implementation, using properties of the abstract model as lemmas. In addition to simplifying the proof, abstract models provide another useful strategy to hide functions, properties or theories that break decidability. This approach, in combination with theory hiding, was used to verify implementations of distributed consensus protocols [28]. Modularity provides the primary means in Ivy of keeping the automated reasoning decidable.

```
1  isolate foo = {
2      type t
3      action ub(x:t) returns (y:t)
4
5      specification {
6          relation seen(X:t)
7          property ∀X : t.¬(X < X)
8          after init {
9              seen(X) := false;
10         }
11         before ub {
12             require x ≥ 0;
13         }
14         after ub {
15             seen(x) := true;
16             ensure seen(X) → X ≤ y;
17         }
18     }
19     implementation {
20         var max : t
21         after init {
22             max := 0;
23         }
24         implement ub {
25             max := x if x > max else max;
26             y := max;
27         }
28         interpret t → int
29         invariant seen(X) → X ≤ max
30     }
31 }
```

Fig. 2. Example of an Ivy isolate.

3 Verification Tactics

Ivy provides a range of automated tactics for discharging proof goals that are selected for their relatively predictable and stable performance, and for the ability to fail transparently.

3.1 Invariant Checking with SMT

The default tactic for proving safety properties is proof by inductive invariant, using the SMT solver Z3 [21]. For example, in Fig. 2, the guarantee at line 16 is proved using the auxiliary inductive invariant at line 29. The invariant relates the hidden implementation state variable 'max' with the visible specification state variable 'seen'. An invariant is a property that is required to hold only between executions of actions of the isolate. That is, actions may temporarily violate an invariant, but must re-establish it before terminating. The VC (verification condition) for the isolate holds if all invariants are established by the intializers and preserved by the interface actions, and if the invariant implies that no assertion in the code fails. These conditions are verified modulo the visible theories.

Before attempting to prove the VC, the invariance tactic sends it to the *fragment checker*, which determines whether the VC is in a logical fragment called FAU [12] for which Z3 is a decision procedure. If the VC is not in FAU, Ivy provides an explanation to the user, by pointing to formulas that create a *function cycle* or that violate rules for the use of quantifiers and interpreted operators of the visible theories. A function cycle is a cycle in a graph whose vertices are types and whose edges are functions (including Skolem functions). This transparent mode of failure helps the user to reorganize the proof to keep the VC's in the decidable fragment.

If a VC in the decidable fragment is false, Z3 fails transparently, producing a true finite counter-model, which is in turn translated into an execution trace

that violates an invariant or guarantee. Ivy provides a graphical interactive tool to help the user in strengthening invariants [25] based on counterexamples. If the VC is valid, the tactic discharges the proof goal, returning the empty set of subgoals.

3.2 Eager Abstraction and Model Checking

An alternative tactic to prove safety properties is model checking with eager abstraction [19]. This technique allows parameterized and infinite-state systems to be verified with a finite-state model checker. The tactic first propositionally strengthens the symbolic transition relation by adding instances of axioms of the logic and theories, or of proved properties. It then propositionally abstracts the transition relation by converting the atomic predicates to Boolean variables. The resulting finite-state abstraction is verified by the ABC model checker [8]. If the property is false, the user is presented with an abstract counterexample expressed in terms of the truth values of the atomic propositions. The user may refine the abstraction by adding instantiation terms or auxiliary invariants. In [19] it was shown that this technique can reduce the burden of constructing auxiliary invariants, simplifying the overall proof of distributed protocols. As an example, the isolate of Fig. 2 can be proved without the auxiliary invariant. With eager abstraction, one need not be concerned with function cycles, but on the other hand, diagnosing abstract counterexamples can be challenging.

This approach is consistent with Ivy's philosophy of using stable and transparent automation, since the finite-state model checker has a single-exponential upper complexity bound and terminates with a proof or a counterexample. This is in contrast to more powerful proof engines such as Horn solvers [6] that suffer from unpredictable divergence. In practice, although eager abstraction is not fully automated, it can handle problems that are substantially beyond the capabilities of current Horn solvers.

3.3 Liveness-to-Safety Transformation

Ivy supports proofs of temporal properties, e.g., liveness properties, via a liveness-to-safety transformation. Temporal properties are specified in first-order linear temporal logic (FO-LTL). The liveness-to-safety tactic reduces a temporal proof goal into a safety proof goal, which can then be proven using an inductive invariant. For finite-state or parameterized systems, any temporal property can be proven by showing the absence of fair cycles, which is a safety property [27]. For infinite-state systems such an argument is not sound, and Ivy implements *dynamic abstraction* which generalizes the notion of fair cycles to infinite-state systems in a sound and powerful way [23,24]. With dynamic abstraction, Ivy's liveness-to-safety tactic supports temporal proofs of infinite-state systems, including both distributed systems with infinite-state per process and systems with *unbounded parallelism*, where new processes can be dynamically created so an infinite trace may involve infinite set of processes.

```
1  isolate bar = {
2      finite type t
3      action step(x:t)
4      specification {
5          relation pending(X:t)
6          instance enter : signal
7
8          after init {
9              pending(X) := true;
10         }
11         before step {
12             require pending(x);
13             call enter.raise;
14             pending(x) := false;
15         }
16         temporal property (□◇ enter.now) →
17             ◇ ∀X. ¬pending(X)
18         proof {
19             tactic l2s with
20             invariant ◇ enter.now
21             invariant ($was$ ¬pending(X)) → ¬pending(X)
22             invariant ($happened$ enter.now) →
23                 ∃X. ($was$ pending(X)) ∧ ¬pending(X)
24         }
25     }
26 }
```

Fig. 3. Example of an Ivy isolate with a temporal property.

The liveness-to-safety tactic fits within Ivy's philosophy of using decidable reasoning. The more standard way of proving liveness properties is to use ranking functions, but for distributed systems, the required rankings often involve cardinalities of sets defined via first-order formulas, resulting in verification conditions that fall outside FAU and other decidable fragments. In contrast, the transformation to safety based on fair cycles and dynamic abstraction results in verification conditions which are often in the FAU fragment. Furthermore, since the temporal proof is transformed to a safety verification problem, it is possible to leverage for liveness proofs all the tactics and mechanisms that Ivy contains for safety verification.

When the liveness-to-safety tactic is applied, Ivy constructs a symbolic *cycle detection transition system*, which tracks fairness constraints and includes a *shadow* or *saved copy* of the state variables, similar to [5]. For finite-state or parameterized systems, it is enough to show that it is not possible to revisit the saved state while satisfying all fairness constraints. This can be shown by an inductive invariant, and Ivy contains special syntax for writing the invariant of the cycle detection system (e.g., to access the saved copy of state variables). For infinite-state systems, Ivy's cycle detection system includes dynamic abstraction, and invariants may also refer to the state of the abstraction [23].

Figure 3 shows an example of a simple liveness proof of an abstract model in Ivy. The type t (line 2) is declared as finite, which means it is sound to use a fair cycle argument without dynamic abstraction. The specification state of the system consists of a single unary relation, pending, which is initialized to true for all values of type t. The step action (line 11) removes a single value from the pending relation. This can model, e.g., execution of tasks from a finite pool of pending tasks. The temporal property that we prove (line 16) is that if step is called infinitely often, then eventually nothing is pending. At line 13, we detect the call by raising a flag enter.now. The proof applies the liveness-to-safety (l2s) tactic (line 19), and supplies inductive invariants for the cycle detection system. The special operators was and $happened$ are used to refer to the saved state, and the fairness constraints, respectively. The crux of the invariant is that after

```
1  axiom eid(X) = eid(Y) → X = Y
2  axiom mgr(X, Y) ∧ mgr(X, Z) → Y = Z
3  explicit axiom [mgr_total] ∃Y. mgr(X, Y)
4  axiom mgr(X, X) → X = ceo
5
6  invariant mgr(X, Y) ∧ scanned(Y) → mid(X) = eid(Y)
7
8  action get_mid(x:emp) returns (res:id) = {
9      require ∀Y.scanned(Y);
10     res := mid(x);
11     ensure x ≠ ceo → res ≠ eid(x);
12     proof {
13         assume mgr_total with X = x
14     }
15 }
```

Fig. 4. Example of manual quantifier instantiation with a tactic

enter.now has happened, there is some element which was pending in the saved state and is not pending anymore, showing that the system has no fair cycle.

3.4 Logical Tactics

Though most of a proof in Ivy is done with the above automated proof tactics, there are occasional situations in which a small amount of detailed manually-guided proof is needed, or is preferable to restructuring the proof. For this purpose, Ivy provides logical proof tactics that can be applied to properties, invariants or code assertions, either to complete the proof or to reduce it to subgoals that can be discharged by the automated tactics. A simple example is shown in Fig. 4. Here, $\mathrm{mgr}(X, Y)$ indicates that the manager of employee X is Y and $\mathrm{eid}(X)$ is the employee id of X. We assume that employee ids are unique, each employee has exactly one manager and that only the CEO is her own manager (lines 1 to 4). Action get_mid(x) returns the id of the manager of employee x. For this purpose, a procedure (not shown) scans the employees m and sets $\mathrm{mid}(x) = \mathrm{eid}(m)$ for each x managed by m, establishing the invariant at line 6. Action get_mid(x) requires that all employees have been scanned and ensures that the return value is not the id of x, unless x is the CEO.

Axiom mgr_total states that for all employees there exists a manager (the universal quantifier on X is implicit). Ivy complains that this quantifier alternation puts the VC outside the decidable fragment. We can solve this with a manual quantifier instantiation. We first tag the axiom *explicit*, meaning that it is not used by the default tactic. We then apply the tactic 'assume' (line 13) to instantiate this axiom for $X = x$. The resulting assumption $\exists Y.\mathrm{mgr}(x, Y)$ has no alternation. The modified proof goal is discharged by the default tactic using Z3. Ivy's proof engine is based on the $\lambda\Pi$ calculus [13] and a deterministic second-order matching algorithm [30]. The Ivy standard library uses this framework to define proof rules for natural deduction, similarly to Isabelle/FOL [26]. Logical tactics also make it possible to perform theory reasoning outside the decidable fragment, for example, applying the Peano induction axiom.

4 Light-Weight Formal Methods

4.1 Compositional Specification-Based Testing

Before attempting a formal proof that an isolate satisfies its specification, it is useful to debug it using testing. For this purpose, Ivy provides compositional specification-based testing. The testers that Ivy produces generate randomized input sequences for an isolate that satisfy its assumptions and check the outputs against the isolate's guarantees. This is similar in principle to specification-based testing tools such as QuickCheck [9], but is reactive and compositional. Compositionality provides a kind of completeness for unit testing. That is, if a system fails its specification, then there is a local test of some component that fails. Unlike QuickCheck, Ivy does not require the user to provide generators for datatypes, instead relying on SMT solving for this purpose. Ivy can also be used to generate specification-based tests for hardware or software systems not written in Ivy. For example, it has been used to find bugs in memory hierarchy components for RISC-V processors [18], and the QUIC secure Internet transport protocol [20].

4.2 Bounded and Finite-State Model Checking

For debugging, Ivy supports bounded model checking. This is decidable if the VC's are in the decidable fragment. It also allows uninterpreted types to be finitely instantiated, allowing under-approximate model checking in the style of TLC [31].

5 Extracting Efficient Executable Code

Compilation. The implementation part of an Ivy program can be extracted as executable code in C++. To be extractable, the implementation must satisfy certain computability conditions, for example that all quantifiers in conditionals be bounded. For functions, the compiler can choose among several representations: a closure, a dense representation as an array, or a sparse representation as a hash table. The dense representation is unboxed, allowing a cache-efficient contiguous representation of an array of structures and reducing allocation overhead.

Because there are no references in Ivy, there is a risk of copying large structures passed as arguments. However, the lack of aliasing makes it relatively easy for the compiler to detect linear use of data, allowing call and return by reference in the extracted code, and in-place update of structures. Subtype polymorphism in Ivy is implemented by the compiler using smart pointers, allowing structure sharing (and potentially copy-on-write, though this is not yet implemented). In addition, the compiler borrows a technique from the Rust language [22] to introduce references. Consider the Ivy code on the left of Fig. 5 that looks up a value in a map, operates on it, then writes it back into the map. The compiler recognizes this as an instance of the "borrowing" pattern and renders it as the C++ code on the right, which operates on the value in the map by reference.

```
b := m(x);
b := f(b);
m(x) := b;
```

```
auto &b = m[x];
f(b);
```

Fig. 5. Updating a map in place using the borrow pattern.

This is possible because the of lack of aliasing and the fact that the compiler understands the underlying data structures. A C++ compiler cannot accomplish this optimization because of the difficulty of pointer analysis in the map implementation and the called operator f. Benchmarks of an older Ivy compiler [28] on distributed protocols showed comparable performance to implementation in OCaml and Go, though Ivy is purely value-based, while these languages support references.

Concurrency. Although Ivy is a synchronous reactive language, the compiler can extract parameterized distributed programs from Ivy programs in a sound way. In a parameterized module, each action and state variable has a first parameter representing a *location*. The compiler verifies that different locations do not interfere with each-other, and then extracts an executable process that takes its location as a parameter. Ivy guarantees that executing the locations concurrently is observably equivalent sequential execution, based on a left-mover/right-mover argument [15,28].

Run-Time Support. Ivy provide a standard library that includes useful abstractions, such ordered datatypes and arrays, as well as formally specified interfaces to networking services provided by operating systems. In addition, the compiler automatically generates marshaling and unmarshaling code for user-defined datatypes. These facilities make it relatively straightforward to implement verified networked protocols in Ivy.

6 Conclusion

Ivy has been designed to provide predictability, stability and transparency in the process of developing verified systems. For this purpose, it integrates a collection of verification techniques that provide these properties, while attempting to maximize the expressiveness of the language, the degree of proof automation, and the efficiency of extracted code. By setting the division of labor between the human and automated provers appropriately, it aims to increase the productivity of the overall process of formal development.

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Reasoning over Permissions Regions in Concurrent Separation Logic

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Abstract. We propose an extension of separation logic with fractional permissions, aimed at reasoning about concurrent programs that share arbitrary *regions* or data structures in memory. In existing formalisms, such reasoning typically either fails or is subject to stringent side conditions on formulas (notably *precision*) that significantly impair automation. We suggest two formal syntactic additions that collectively remove the need for such side conditions: first, the use of both "weak" and "strong" forms of separating conjunction, and second, the use of nominal labels from hybrid logic. We contend that our suggested alterations bring formal reasoning with fractional permissions in separation logic considerably closer to common pen-and-paper intuition, while imposing only a modest bureaucratic overhead.

Keywords: Separation logic · Permissions · Concurrency · Verification

1 Introduction

Concurrent separation logic (CSL) is a version of separation logic designed to enable compositional reasoning about concurrent programs that manipulate memory possibly shared between threads [6,26]. Like standard separation logic [28], CSL is based on *Hoare triples* $\{A\}\,C\,\{B\}$, where C is a program and A and B are formulas (called the *precondition* and *postcondition* of the code respectively). The heart of the formalism is the following *concurrency rule*:

$$\frac{\{A_1\}\,C_1\,\{B_1\} \quad \{A_2\}\,C_2\,\{B_2\}}{\{A_1 \circledast A_2\}\,C_1 \,||\, C_2\,\{B_1 \circledast B_2\}}$$

where $\circledast$ is a so-called *separating conjunction*. This rule says that if two threads C_1 and C_2 are run on spatially separated resources $A_1 \circledast A_2$ then the result will be the spatially separated result, $B_1 \circledast B_2$, of running the two threads individually.

However, since many or perhaps even most interesting concurrent programs do share some resources, $\circledast$ typically does not denote strict disjoint separation of memories, as it does in standard separation logic (where it is usually written as $*$).

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Instead, it usually denotes a weaker sort of "separation" designed to ensure that the two threads at least cannot interfere with each others' data. This gives rise to the idea of *fractional permissions*, which allow us to divide writeable memory into multiple read-only copies by adding a permission value to each location in heap memory. In the usual model, due to Boyland [5], permissions are rational numbers in the half-open interval $(0, 1]$, with 1 denoting the write permission, and values in $(0, 1)$ denoting read-only permissions. We write the formula A^π, where π is a permission, to denote a "π share" of the formula A. For example, $(x \mapsto a)^{0.5}$ (typically written as $x \overset{0.5}{\mapsto} a$ for convenience) denotes a "half share" of a single heap cell, with address x and value a. The separating conjunction $A \circledast B$ then denotes heaps realising A and B that are "compatible", rather than disjoint: where the heaps overlap, they must agree on the data value, and one adds the permissions at the overlapping locations [4]. E.g., at the logical level, we have the entailment:

$$x \overset{0.5}{\mapsto} a \circledast x \overset{0.5}{\mapsto} b \models a = b \wedge x \mapsto a. \tag{1}$$

Happily, the concurrency rule of CSL is still sound in this setting (see e.g. [29]).

However, the use of this weaker notion of separation $\circledast$ causes complications for formal reasoning in separation logic, especially if one wishes to reason over arbitrary regions of memory rather than individual pointers. There are two particular difficulties, as identified by Le and Hobor [24]. The first is that, since $\circledast$ denotes possibly-overlapping memories, one loses the main useful feature of separation logic: its nonambiguity about separation, which means that desirable entailments such as $A^{0.5} \circledast B^{0.5} \models (A \circledast B)^{0.5}$ turn out to be false. E.g.:

$$x \overset{0.5}{\mapsto} a \circledast y \overset{0.5}{\mapsto} b \not\models (x \mapsto a \circledast y \mapsto b)^{0.5}.$$

Here, the two "half-pointers" on the LHS might be aliased ($x = y$ and $a = b$), meaning they are two halves of the same pointer, whereas on the RHS they must be non-aliased (because we cannot combine two "whole" pointers). This ambiguity becomes quite annoying when one adds arbitrary predicate symbols to the logic, e.g. to support inductively defined data structures.

The second difficulty is that although recombining single pointers is straightforward, as indicated by Eq. (1), recombining the shares of arbitrary formulae is challenging. E.g., $A^{0.5} \circledast A^{0.5} \not\models A$, as shown by the counterexample

$$(x \mapsto 1 \vee y \mapsto 2)^{0.5} \circledast (x \mapsto 1 \vee y \mapsto 2)^{0.5} \not\models x \mapsto 1 \vee y \mapsto 2.$$

The LHS can be satisfied by a heap with a 0.5-share of x and a 0.5-share of y, whereas the RHS requires a full (1) share of either x or y.

Le et al. [24] address these problems by a combination of the use of *tree shares* (essentially Boolean binary trees) rather than rational numbers as permissions, and semantic restrictions on when the above sorts of permissions reasoning can be applied. For example, recombining permissions ($A^{0.5} \circledast A^{0.5} \models A$) is permitted only when the formula is *precise* in the usual separation logic sense (cf. [28]). The chief drawback with this approach is the need to repeatedly check these side

conditions on formulas when reasoning, as well as that said reasoning cannot be performed on imprecise formulas.

Instead, we propose to resolve these difficulties by a different, two-pronged extension to the syntax of the logic. First, we propose that the usual "strong" separating conjunction $*$, which enforces the strict disjointness of memory, *should be retained* in the formalism in addition to the weaker $\circledast$. The stronger $*$ supports entailments such as $A^{0.5} * B^{0.5} \models (A * B)^{0.5}$, which does not hold when $\circledast$ is used instead. Second, we introduce *nominal labels* from hybrid logic (cf. [3,10]) to remember that two copies of a formula have the same origin. We write a nominal α to denote a unique heap, in which case entailments such as $(\alpha \wedge A)^{0.5} \circledast (\alpha \wedge A)^{0.5} \models \alpha \wedge A$ become valid. We remark that labels have been adopted for similar "tracking" purposes in several other separation logic proof systems [10,21,23,25].

The remainder of this paper aims to demonstrate that our proposed extensions are (i) weakly *necessary*, in that expected reasoning patterns fail under the usual formalism, (ii) *correct*, in that they recover the desired logical principles, and (iii) *sufficient* to verify typical concurrent programming patterns that use sharing. Section 2 gives some simple examples that motivate our extensions. Section 3 then formally introduces the syntax and semantics of our extended formalism. In Sect. 4 we show that our logic obeys the logical principles that enable us to reason smoothly with fractional permissions over arbitrary formulas, and in Sect. 5 we give some longer worked examples. Finally, in Sect. 6 we conclude and discuss directions for future work.

2 Motivating Examples

In this section, we aim to motivate our extensions to separation logic with permissions by showing, firstly, how the failures of the logical principles described in the introduction actually arise in program verification examples and, secondly, how these failures are remedied by our proposed changes.

The overall context of our work is reasoning about concurrent programs that share some data structure or region in memory, which can be described as a formula in the assertion language. If A is such a formula then we write A^π to denote a "π share" of the formula A, meaning informally that all of the pointers in the heap memory satisfying A are owned with share π. The main question then becomes how this notion interacts with the separating conjunction $\circledast$. There are two key desirable logical equivalences:

$$(A \circledast B)^\pi \equiv A^\pi \circledast B^\pi \tag{I}$$

$$A^{\pi \oplus \sigma} \equiv A^\pi \circledast A^\sigma \tag{II}$$

Equivalence (I) describes distributing a fractional share over a separating conjunction, whereas equivalence (II) describes combining two pieces of a previously split resource. Both equivalences are true in the $\models$ direction but, as we have seen in the Introduction, false in the $=\!\!|$ one. Generally speaking, $\circledast$ is like Humpty Dumpty: easy to break apart, but not so easy to put back together again.

The key to understanding the difficulty is the following equivalence:

$$x \overset{\pi}{\mapsto} a \circledast y \overset{\sigma}{\mapsto} b \;\equiv\; (x \overset{\pi}{\mapsto} a * y \overset{\sigma}{\mapsto} b) \vee (x = y \wedge a = b \wedge x \overset{\pi \oplus \sigma}{\mapsto} a)$$

In other words, either x and y are not aliased, or they *are* aliased and the permissions combine (the additive operation $\oplus$ on rational shares is simply normal addition when the sum is ≤ 1 and undefined otherwise). This disjunction undermines the notational economies that have led to separation logic's great successes in scalable verification [11]; in particular, (I) fails because the left disjunct might be true, and (II) fails because the right disjunct might be. At a high level, $\circledast$ is a bit too easy to introduce, and therefore also a bit too hard to eliminate.

2.1 Weak vs. Strong Separation and the Distribution Principle

One of the challenges of the weak separating conjunction $\circledast$ is that it interacts poorly with inductively defined predicates. Consider porting the usual separation logic definition of a possibly-cyclic linked list segment from x to y from a sequential setting to a concurrent one by a simple substitution of $\circledast$ for $*$:

$$\mathsf{ls}\, x\, y \;=_{\text{def}}\; (x = y \wedge \mathsf{emp}) \vee (\exists z.\; x \mapsto z \circledast \mathsf{ls}\, z\, y).$$

Now consider a simple recursive procedure `foo(x,y)` that traverses a linked list segment from `x` to `y`:

```
foo(x,y) { if x=y then return; else foo([x],y); }
```

It is easy to see that `foo` leaves the list segment unchanged, and therefore satisfies the following Hoare triple:

$$\{(\mathsf{ls}\, x\, y)^{0.5}\}\ \texttt{foo(x,y);}\ \{(\mathsf{ls}\, x\, y)^{0.5}\}.$$

The intuitive proof of this fact would run approximately as follows:

$\{(\mathsf{ls}\, x\, y)^{0.5}\}$ `foo(x,y) {`

`if x=y then return;` $\{(\mathsf{ls}\, x\, y)^{0.5}\}$

`else` $\{x \neq y \wedge (x \mapsto z \circledast \mathsf{ls}\, z\, y)^{0.5}\}$

$\{x \overset{0.5}{\mapsto} z \circledast (\mathsf{ls}\, z\, y)^{0.5}\}$

`foo([x],y);` $\{x \overset{0.5}{\mapsto} z \circledast (\mathsf{ls}\, z\, y)^{0.5}\}$

$\{(x \mapsto z \circledast \mathsf{ls}\, z\, y)^{0.5}\}$

$\{(\mathsf{ls}\, x\, y)^{0.5}\}$

`}` $\{(\mathsf{ls}\, x\, y)^{0.5}\}$

However, because of the use of $\circledast$, the highlighted inference step is not sound:

$$x \overset{0.5}{\mapsto} z \circledast (\mathsf{ls}\, z\, y)^{0.5} \not\models (x \mapsto z \circledast \mathsf{ls}\, z\, y)^{0.5}. \tag{2}$$

To see this, consider a heap with the following structure, viewed in two ways:

$$x \overset{0.5}{\mapsto} z \circledast z \overset{0.5}{\mapsto} x \circledast x \overset{0.5}{\mapsto} z \quad = \quad x \mapsto z \circledast z \overset{0.5}{\mapsto} x$$

This heap satisfies the LHS of the entailment in (2), as it is the $\circledast$-composition of a 0.5-share of $x \mapsto z$ and a 0.5-share of $\mathsf{ls}\, z\, z$, a cyclic list segment from z back to itself (note that here $z = y$). However, it does not satisfy the RHS, since it is not a 0.5-share of the $\circledast$-composition of $x \mapsto z$ with $\mathsf{ls}\, z\, z$, which would require the pointer to be disjoint from the list segment.

The underlying reason for the failure of this example is that, in going from $(x \mapsto z \circledast \mathsf{ls}\, z\, z)^{0.5}$ to $x \overset{0.5}{\mapsto} z \circledast (\mathsf{ls}\, z\, z)^{0.5}$, we have lost the information that the pointer and the list segment are actually disjoint. This is reflected in the general failure of the distribution principle $A^\pi \circledast B^\pi \models (A \circledast B)^\pi$, of which the above is just one instance. Accordingly, our proposal is that the "strong" separating conjunction $*$ from standard separation logic, which forces disjointness of the heaps satisfying its conjuncts, should *also* be retained in the logic alongside $\circledast$, on the grounds that (II) *is* true for the stronger connective:

$$(A * B)^\pi \equiv A^\pi * B^\pi. \tag{3}$$

If we then define our list segments using $*$ in the traditional way, namely

$$\mathsf{ls}\, x\, y \;=_{\text{def}}\; (x = y \wedge \mathsf{emp}) \vee (\exists z.\; x \mapsto z * \mathsf{ls}\, z\, y),$$

then we can observe that this second definition of ls is identical to the first on permission-free formulas, since $\circledast$ and $*$ coincide in that case. However, when we replay the verification proof above with the new definition of ls, every $\circledast$ in the proof above becomes a $*$, and the proof then becomes sound. Nevertheless, we can still use $\circledast$ to describe permission-decomposition of list segments at a higher level; e.g., $\mathsf{ls}\, x\, y$ can still be decomposed as $(\mathsf{ls}\, x\, y)^{0.5} \circledast (\mathsf{ls}\, x\, y)^{0.5}$.

2.2 Nominal Labelling and the Combination Principle

Unfortunately, even when we use the strong separating conjunction $*$ to define list segments ls, a further difficulty still remains. Consider a simple concurrent program that runs two copies of `foo` in parallel on the same list segment:

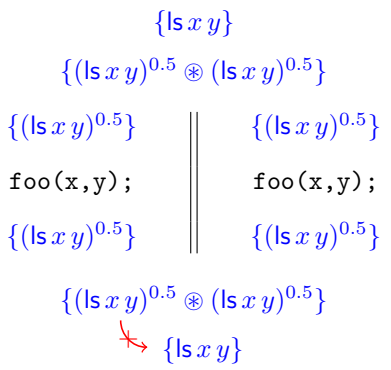
```
foo(x,y); || foo(x,y);
```

Since `foo` only reads from its input list segment, and satisfies the specification $\{(\mathsf{ls}\, x\, y)^{0.5}\}$ `foo(x,y);` $\{(\mathsf{ls}\, x\, y)^{0.5}\}$, this program satisfies the specification

$$\{\mathsf{ls}\, x\, y\}\ \texttt{foo(x,y);}\ \|\ \texttt{foo(x,y);}\ \{\mathsf{ls}\, x\, y\}.$$

Now consider constructing a proof of this specification in CSL. First we view the list segment $\mathsf{ls}\, x\, y$ as the $\circledast$-composition of two read-only copies, with permission 0.5 each; then we use CSL's concurrency rule (see Sect. 1) to compose the

specifications of the two threads; last we recombine the two read-only copies to obtain the original list segment. The proof diagram is as follows:



However, again, the highlighted inference step in this proof is not correct:

$$(\mathsf{ls}\, x\, y)^{0.5} \circledast (\mathsf{ls}\, x\, y)^{0.5} \not\models \mathsf{ls}\, x\, y. \tag{4}$$

A countermodel is a heap with the following structure, again viewed in two ways:

$$(x \overset{0.5}{\mapsto} y \circledast y \overset{0.5}{\mapsto} y) \circledast x \overset{0.5}{\mapsto} y \quad = \quad x \mapsto y \circledast y \overset{0.5}{\mapsto} y$$

According to the first view of such a heap, it satisfies the LHS of (4), as it is the $\circledast$-composition of two 0.5-shares of $\mathsf{ls}\, x\, y$ (one of two cells, and one of a single cell). However, it does not satisfy $\mathsf{ls}\, x\, y$, since that would require every cell in the heap to be owned with permission 1.

Like in our previous example, the reason for the failure of this example is that we have lost information. In going from $\mathsf{ls}\, x\, y$ to $(\mathsf{ls}\, x\, y)^{0.5} \circledast (\mathsf{ls}\, x\, y)^{0.5}$, we have forgotten that the two formulas $(\mathsf{ls}\, x\, y)^{0.5}$ are in fact *copies of the same region*. For formulas A that are *precise* in that they uniquely describe part of any given heap [12], e.g. formulas $x \mapsto a$, this loss of information does not happen and we do have $A^{0.5} \circledast A^{0.5} \models A$; but for non-precise formulas such as $\mathsf{ls}\, x\, y$, this principle fails.

However, we regard this primarily as a technical shortcoming of the formalism, rather than a failure of our intuition. It *ought* to be true that we can take any region of memory, split it into two read-only copies, and then later merge the two copies to re-obtain the original region. Were we conducting the above proof on pen and paper, we would very likely explain the difficulty away by adopting some kind of labelling convention, allowing us to remember that two formulas have been obtained from the same memory region by dividing permissions.

In fact, that is almost exactly our proposed remedy to the situation. We introduce *nominals*, or *labels*, from hybrid logic, where a nominal α is interpreted as denoting a unique heap. Any formula of the form $\alpha \wedge A$ is then precise (in the above sense), and so obeys the combination principle

$$(\alpha \wedge A)^{\pi} \circledast (\alpha \wedge A)^{\sigma} \models (\alpha \wedge A)^{\sigma \oplus \pi}, \tag{5}$$

where $\oplus$ is addition on permissions. Thus we can repair the faulty CSL proof above by replacing every instance of the formula $\mathsf{ls}\,x\,y$ by the "labelled" formula $\alpha \wedge \mathsf{ls}\,x\,y$ (and adding an initial step in which we introduce the fresh label α).

2.3 The Jump Modality

However, this is not quite the end of the story. Readers may have noticed that replacing $\mathsf{ls}\,x\,y$ by the "labelled" version $\alpha \wedge \mathsf{ls}\,x\,y$ also entails establishing a slightly stronger specification for the function `foo`, namely:

$$\{(\alpha \wedge \mathsf{ls}\,x\,y)^{0.5}\}\ \texttt{foo(x,y);}\ \{(\alpha \wedge \mathsf{ls}\,x\,y)^{0.5}\}.$$

This introduces an extra difficulty in the proof (cf. Sect. 2.1); at the recursive call to `foo([x],y)`, the precondition now becomes $\alpha^{0.5} \wedge (x \overset{0.5}{\mapsto} z * (\mathsf{ls}\,z\,y)^{0.5}))$, which means that we cannot apply separation logic's *frame rule* [32] to the pointer formula without first weakening away the label-share $\alpha^{0.5}$.

For this reason, we shall also employ hybrid logic's "jump" modality $@_{\_}$, where the formula $@_\alpha A$ means that A is true of the heap denoted by the label α. In the above, we can introduce labels β and γ for the list components $x \mapsto z$ and $\mathsf{ls}\,z\,y$ respectively, whereby we can represent the decomposition of the list by the assertion $@_\alpha(\beta * \gamma)$. Since this is a *pure* assertion that does not depend on the heap, it can be safely maintained when applying the frame rule, and used after the function call to restore the label α, using the easily verifiable fact that

$$@_\alpha(\beta * \gamma) \wedge (\beta * \gamma) \models \alpha.$$

Similar reasoning over labelled decompositions of data structures is seemingly necessary whenever treating recursion; we return to it in more detail in Sect. 5.

3 Separation Logic with Labels and Permissions ($\mathsf{SL}_{\mathsf{LP}}$)

Following the motivation given in the previous section, here we give the syntax and semantics of a separation logic, $\mathsf{SL}_{\mathsf{LP}}$, with permissions over arbitrary formulas, making use of both strong *and* weak separating conjunctions, and nominal labels (from hybrid logic [3,10]). First, we define a suitable notion of permissions and associated operations.

Definition 3.1. *A* permissions algebra *is a tuple* $\langle \mathsf{Perm}, \oplus, \otimes, 1 \rangle$*, where* Perm *is a set (of "permissions"),* $1 \in \mathsf{Perm}$ *is called the* write permission*, and* $\oplus$ *and* $\otimes$ *are respectively partial and total binary functions on* Perm*, satisfying associativity, commutativity, cancellativity and the following additional axioms:*

$\pi_1 \oplus \pi_2 \neq \pi_2$	*(non-zero)*
$\forall \pi.\ \pi \oplus 1$ *is undefined*	*(top)*
$\forall \pi.\ \exists \pi_1, \pi_2.\ \pi = \pi_1 \oplus \pi_2$	*(divisibility)*
$(\pi_1 \oplus \pi_2) \otimes \pi = (\pi_1 \otimes \pi) \oplus (\pi_2 \otimes \pi)$	*(left-dist)*

The most common example of a permissions algebra is the Boyland fractional permission model $\langle (0,1] \cap \mathbb{Q}, \oplus, \times, 1 \rangle$, where permissions are rational numbers in $(0,1]$, $\times$ is standard multiplication, and $\oplus$ is standard addition but undefined if $p + p' > 1$. From now on, we assume a fixed but arbitrary permissions algebra.

With the permissions structure in place, we can now define the syntax of our logic. We assume disjoint, countably infinite sets Var of variables, Pred of predicate symbols (with associated arities) and Label of labels.

Definition 3.2. *We define* formulas *of* $\mathsf{SL_{LP}}$ *by the grammar:*

$$\begin{array}{lll} A ::= x = y \mid \neg A \mid A \wedge A \mid A \vee A \mid A \to A & & \textit{(pure)} \\ \quad \mid \mathsf{emp} \mid x \mapsto y \mid P(\mathbf{x}) \mid A * A \mid A \circledast A \mid A \mathrel{-\!\!*} A \mid A \mathrel{-\!\!\circledast} A & & \textit{(spatial)} \\ \quad \mid A^{\pi} \mid \alpha \mid @_{\alpha} A & & \textit{(perms/labels)} \end{array}$$

where x, y range over Var*, π ranges over* Perm*, P ranges over* Pred*, α ranges over* Label *and* $\mathbf{x}$ *ranges over tuples of variables of length matching the arity of the predicate symbol P. We write $x \overset{\pi}{\mapsto} y$ for $(x \mapsto y)^{\pi}$, and $x \neq y$ for $\neg(x = y)$.*

The "magic wands" $\mathrel{-\!\!*}$ and $\mathrel{-\!\!\circledast}$ are the implications adjoint to $*$ and $\circledast$, as usual in separation logic. We include them for completeness, but we use $\mathrel{-\!\!*}$ only for fairly complex examples (see Sect. 5.3) and in fact do not use $\mathrel{-\!\!\circledast}$ at all.

Semantics. We interpret formulas in a standard model of stacks and heaps-with-permissions (cf. [4]), except that our models also incorporate a valuation of nominal labels. We assume an infinite set Val of *values* of which an infinite subset $\mathsf{Loc} \subset \mathsf{Val}$ are considered addressable *locations*. A *stack* is as usual a map $s : \mathsf{Var} \to \mathsf{Val}$. A *heap-with-permissions*, which we call a *p-heap* for short, is a finite partial function $h : \mathsf{Loc} \rightharpoonup_{\text{fin}} \mathsf{Val} \times \mathsf{Perm}$ from locations to value-permission pairs. We write $\mathrm{dom}\,(h)$ for the *domain* of h, i.e. the set of locations on which h is defined. Two p-heaps h_1 and h_2 are called *disjoint* if $\mathrm{dom}\,(h_1) \cap \mathrm{dom}\,(h_2) = \emptyset$, and *compatible* if, for all $\ell \in \mathrm{dom}\,(h_1) \cap \mathrm{dom}\,(h_2)$, we have $h_1(\ell) = (v, \pi_1)$ and $h_2(v, \pi_2)$ and $\pi_1 \oplus \pi_2$ is defined. (Thus, trivially, disjoint heaps are also compatible.) We define the multiplication $\pi \cdot h$ of a p-heap h by permission π by extending $\otimes$ pointwise:

$$(\pi \cdot h)(\ell) = (v, \pi \otimes \pi') \quad \Leftrightarrow \quad h(\ell) = (v, \pi').$$

We also assume that each predicate symbol P of arity k is given a fixed interpretation $[\![P]\!] \in (\mathsf{Val}^k \times \mathsf{PHeaps})$, where PHeaps is the set of all p-heaps. Here we allow an essentially free interpretation of predicate symbols, but they could also be given by a suitable inductive definition schema, as is done in many papers on separation logic (e.g. [7,8]). Finally, a *valuation* is a function $\rho : \mathsf{Label} \to \mathsf{PHeaps}$ assigning a single p-heap $\rho(\alpha)$ to each label α.

Definition 3.3 (Strong and weak heap composition). *The* strong composition $h_1 \circ h_2$ *of two disjoint p-heaps h_1 and h_2 is defined as their union:*

$$(h_1 \circ h_2)(\ell) = \begin{cases} h_1(\ell) & \text{if } \ell \notin \mathrm{dom}\,(h_2) \\ h_2(\ell) & \text{if } \ell \notin \mathrm{dom}\,(h_1) \end{cases}$$

$$
\begin{array}{lcl}
s,h,\rho \models x = y & \Leftrightarrow & s(x) = s(y) \\
s,h,\rho \models \neg A & \Leftrightarrow & s,h,\rho \not\models A \\
s,h,\rho \models A \wedge B & \Leftrightarrow & s,h,\rho \models A \text{ and } s,h,\rho \models B \\
s,h,\rho \models A \vee B & \Leftrightarrow & s,h,\rho \models A \text{ or } s,h,\rho \models B \\
s,h,\rho \models A \to B & \Leftrightarrow & s,h,\rho \models A \text{ implies } s,h,\rho \models B \\
s,h,\rho \models \mathsf{emp} & \Leftrightarrow & \mathrm{dom}\,(h) = \emptyset \\
s,h,\rho \models x \mapsto y & \Leftrightarrow & \mathrm{dom}\,(h) = \{s(x)\} \text{ and } h(s(x)) = (s(y),1) \\
s,h,\rho \models P(\mathbf{x}) & \Leftrightarrow & (s(\mathbf{x}),h) \in [\![P]\!] \\
s,h,\rho \models A * B & \Leftrightarrow & \exists h_1,h_2.\ h = h_1 \circ h_2 \text{ and } s,h_1,\rho \models A \text{ and } s,h_2,\rho \models B \\
s,h,\rho \models A \circledast B & \Leftrightarrow & \exists h_1,h_2.\ h = h_1 \mathbin{\overline{\circ}} h_2 \text{ and } s,h_1,\rho \models A \text{ and } s,h_2,\rho \models B \\
s,h,\rho \models A \mathrel{-\!\!*} B & \Leftrightarrow & \forall h'.\ \text{if } h \circ h' \text{ defined and } s,h',\rho \models A \text{ then } s,h \circ h',\rho \models B \\
s,h,\rho \models A \mathrel{-\!\!\circledast} B & \Leftrightarrow & \forall h'.\ \text{if } h \mathbin{\overline{\circ}} h' \text{ defined and } s,h',\rho \models A \text{ then } s,h \mathbin{\overline{\circ}} h',\rho \models B \\
s,h,\rho \models A^{\pi} & \Leftrightarrow & \exists h'.\ h = \pi \cdot h' \text{ and } s,h',\rho \models A \\
s,h,\rho \models \alpha & \Leftrightarrow & h = \rho(\alpha) \\
s,h,\rho \models @_{\alpha} A & \Leftrightarrow & s,\rho(\alpha),\rho \models A
\end{array}
$$

Fig. 1. Definition of the satisfaction relation $s,h,\rho \models A$ for $\mathsf{SL}_{\mathsf{LP}}$.

If h_1 and h_2 are not disjoint then $h_1 \circ h_2$ is undefined.

The weak composition *$h_1 \mathbin{\overline{\circ}} h_2$ of two compatible p-heaps h_1 and h_2 is defined as their union, adding permissions at overlapping locations:*

$$
(h_1 \mathbin{\overline{\circ}} h_2)(\ell) = \begin{cases} (v, \pi_1 \oplus \pi_2) & \text{if } h_1(\ell) = (v,\pi_1) \text{ and } h_2(\ell) = (v,\pi_2) \\ h_1(\ell) & \text{if } \ell \notin \mathrm{dom}\,(h_2) \\ h_2(\ell) & \text{if } \ell \notin \mathrm{dom}\,(h_1) \end{cases}
$$

If h_1 and h_2 are not compatible then $h_1 \mathbin{\overline{\circ}} h_2$ is undefined.

Definition 3.4. *The satisfaction relation $s,h,\rho \models A$, where s is a stack, h a p-heap, ρ a valuation and A a formula, is defined by structural induction on A in Fig. 1. We write the* entailment *$A \models B$, where A and B are formulas, to mean that if $s,h,\rho \models A$ then $s,h,\rho \models B$. We write the* equivalence *$A \equiv B$ to mean that $A \models B$ and $B \models A$.*

4 Logical Principles of $\mathsf{SL}_{\mathsf{LP}}$

In this section, we establish the main logical entailments and equivalences of $\mathsf{SL}_{\mathsf{LP}}$ that capture the various interactions between the separating conjunctions $\circledast$ and $*$, permissions and labels. As well as being of interest in their own right, many of these principles will be essential in treating the practical verification examples in Sect. 5. In particular, the permission distribution principle for $*$ (cf. (3), Sect. 2) is given in Lemma 4.3, and the permission combination principle for labelled formulas (cf. (5), Sect. 2) is given in Lemma 4.4.

Proposition 4.1. *The following equivalences all hold in* $\mathsf{SL}_{\mathsf{LP}}$*:*

$$\begin{array}{cc} A \circledast B \equiv B \circledast A & A * B \equiv B * A \\ A \circledast (B \circledast C) \equiv (A \circledast B) \circledast C & A * (B * C) \equiv (A * B) * C \\ A \circledast \mathsf{emp} \equiv A & A * \mathsf{emp} \equiv A \end{array}$$

Additionally, the following residuation laws hold:

$$A \models B \mathrel{-\!\!\circledast} C \;\Leftrightarrow\; A \circledast B \models C \quad \text{and} \quad A \models B \mathrel{-\!\!*} C \;\Leftrightarrow\; A * B \models C.$$

In addition, we can always weaken $*$ *to* $\circledast$*:* $A * B \models A \circledast B$*.*

Next, we establish an additional connection between the two separating conjunctions $\circledast$ and $*$.

Lemma 4.2 ($\circledast/*$ distribution). *For all formulas A, B, C and D,*

$$(A \circledast B) * (C \circledast D) \models (A * C) \circledast (B * D). \qquad (\circledast/*)$$

Proof. First we show a corresponding model-theoretic property: for any p-heaps h_1, h_2, h_3 and h_4 such that $(h_1 \mathbin{\overline{\circ}} h_2) \circ (h_3 \mathbin{\overline{\circ}} h_4)$ is defined,

$$(h_1 \mathbin{\overline{\circ}} h_2) \circ (h_3 \mathbin{\overline{\circ}} h_4) = (h_1 \circ h_3) \mathbin{\overline{\circ}} (h_2 \circ h_4) \qquad (6)$$

Since $(h_1 \mathbin{\overline{\circ}} h_2) \circ (h_3 \mathbin{\overline{\circ}} h_4)$ is defined by assumption, we have that $h_1 \mathbin{\overline{\circ}} h_2$ and $h_3 \mathbin{\overline{\circ}} h_4$ are disjoint and that h_1 and h_2, as well as h_3 and h_4 are compatible. In particular, h_1 and h_3 are disjoint, so $h_1 \circ h_3$ is defined; the same reasoning applies to h_2 and h_4. Moreover, since h_1 and h_2 are compatible, $h_1 \circ h_3$ and $h_2 \circ h_4$ must be compatible and so $(h_1 \circ h_3) \mathbin{\overline{\circ}} (h_2 \circ h_4)$ is defined.
Now, writing h for $(h_1 \mathbin{\overline{\circ}} h_2) \circ (h_3 \mathbin{\overline{\circ}} h_4)$, and letting $\ell \in \mathrm{dom}\,(h)$, we have

$$h(\ell) = \begin{cases} h_1(\ell) & \text{if } \ell \notin \mathrm{dom}\,(h_3), \ell \notin \mathrm{dom}\,(h_4) \text{ and } \ell \notin \mathrm{dom}\,(h_2) \\ h_2(\ell) & \text{if } \ell \notin \mathrm{dom}\,(h_3), \ell \notin \mathrm{dom}\,(h_4) \text{ and } \ell \notin \mathrm{dom}\,(h_1) \\ (v, \pi_1 \oplus \pi_2) & \text{if } \ell \notin \mathrm{dom}\,(h_3), \ell \notin \mathrm{dom}\,(h_4) \text{ and } h_1(\ell) = (v, \pi_1) \\ & \text{and } h_2(\ell) = (v, \pi_2) \\ h_3(\ell) & \text{if } \ell \notin \mathrm{dom}\,(h_1), \ell \notin \mathrm{dom}\,(h_2) \text{ and } \ell \notin \mathrm{dom}\,(h_4) \\ h_4(\ell) & \text{if } \ell \notin \mathrm{dom}\,(h_1), \ell \notin \mathrm{dom}\,(h_2) \text{ and } \ell \notin \mathrm{dom}\,(h_3) \\ (u, \pi_3 \oplus \pi_4) & \text{if } \ell \notin \mathrm{dom}\,(h_1), \ell \notin \mathrm{dom}\,(h_2) \text{ and } h_3(\ell) = (u, \pi_3) \\ & \text{and } h_4(\ell) = (u, \pi_4) \end{cases}$$

We can merge the first and fourth cases by noting that $h(\ell) = (h_1 \circ h_3)(\ell)$ if $\ell \notin \mathrm{dom}\,(h_2 \circ h_4)$, and similarly for the second and fifth cases. We can also rewrite the last two cases by observing that $\ell \notin \mathrm{dom}\,(h_3)$ implies $h_1(\ell) = (h_1 \circ h_3)(\ell)$, and so on, resulting in

$$h(\ell) = \begin{cases} (h_1 \circ h_3)(\ell) & \text{if } \ell \notin \mathrm{dom}\,(h_2 \circ h_4) \\ (h_2 \circ h_4)(\ell) & \text{if } \ell \notin \mathrm{dom}\,(h_1 \circ h_3) \\ (w, \sigma_1 \oplus \sigma_2) & \text{if } (h_1 \circ h_3)(\ell) = (w, \sigma_1) \text{ and } (h_2 \circ h_4)(\ell) = (w, \sigma_2) \end{cases}$$

$$= ((h_1 \circ h_3) \mathbin{\overline{\circ}} (h_2 \circ h_4))(\ell).$$

Now we show the main result. Suppose $s, h, \rho \models (A \circledast B) * (C \circledast D)$. This gives us $h = (h_1 \mathbin{\overline{\circ}} h_2) \circ (h_3 \mathbin{\overline{\circ}} h_4)$, where $s, h_1, \rho \models A$ and $s, h_2, \rho \models B$ and $s, h_3, \rho \models C$ and $s, h_4, \rho \models D$. By Eq. (6), we have $h = (h_1 \circ h_3) \mathbin{\overline{\circ}} (h_2 \circ h_4)$, which gives us exactly that $s, h, \rho \models (A * C) \circledast (B * D)$, as required. □

Next, we establish principles for distributing permissions over various connectives, in particular over the strong $*$, stated earlier as (3) in Sect. 2.

Lemma 4.3 (Permission distribution). *The following equivalences hold for all formulas A and B, and permissions π and σ:*

$$\left(A^{\sigma}\right)^{\pi} \equiv A^{\sigma \otimes \pi} \tag{$\otimes$}$$
$$(A \vee B)^{\pi} \equiv A^{\pi} \vee B^{\pi} \tag{$\vee^{\pi}$}$$
$$(A \wedge B)^{\pi} \equiv A^{\pi} \wedge B^{\pi} \tag{$\wedge^{\pi}$}$$
$$(A * B)^{\pi} \equiv A^{\pi} * B^{\pi} \tag{$*^{\pi}$}$$

Proof. We just show the most interesting case, ($*^{\pi}$). First of all, we establish a corresponding model-theoretic property: for any permission π and disjoint p-heaps h_1 and h_2, meaning $h_1 \circ h_2$ is defined,

$$\pi \cdot (h_1 \circ h_2) = (\pi \cdot h_1) \circ (\pi \cdot h_2). \tag{7}$$

To see this, we first observe that for any $\ell \in \mathrm{dom}\,(h_1 \circ h_2)$, we have that either $\ell \in \mathrm{dom}\,(h_1)$ or $\ell \in \mathrm{dom}\,(h_2)$. We just show the case $\ell \in \mathrm{dom}\,(h_1)$, since the other is symmetric. Writing $h_1(\ell) = (v_1, \pi_1)$, and using the fact that $\ell \notin \mathrm{dom}\,(h_2)$,

$$\pi \cdot (h_1 \circ h_2)(\ell) = (v_1, \pi \otimes \pi_1) = (\pi \cdot h_1)(\ell) = ((\pi \cdot h_1) \circ (\pi \cdot h_2))(\ell).$$

Now for the main result, let s, h and ρ be given. We have

$$\begin{aligned}
& s, h, \rho \models (A * B)^{\pi} \\
\Leftrightarrow\ & h = \pi \cdot h' \text{ and } s, h', \rho \models A * B \\
\Leftrightarrow\ & h = \pi \cdot h' \text{ and } h' = h_1 \circ h_2 \text{ and } s, h_1, \rho \models A \text{ and } s, h_2, \rho \models B \\
\Leftrightarrow\ & h = \pi \cdot (h_1 \circ h_2) \text{ and } s, h_1, \rho \models A \text{ and } s, h_2, \rho \models B \\
\Leftrightarrow\ & h = (\pi \cdot h_1) \circ (\pi \cdot h_2) \text{ and } s, h_1, \rho \models A \text{ and } s, h_2, \rho \models B && \text{by (7)} \\
\Leftrightarrow\ & h = h_1' \circ h_2' \text{ and } s, h_1', \rho \models A^{\pi} \text{ and } s, h_2', \rho \models B^{\pi} \\
\Leftrightarrow\ & s, h, \rho \models A^{\pi} * B^{\pi}.
\end{aligned}$$

□

We now establish the main principles for dividing and combining permissions formulas using $\circledast$. As foreshadowed in Sect. 2, the combination principle holds only for formulas that are conjoined with a nominal label (cf. Eq. (5)).

Lemma 4.4 (Permission division and combination). *For all formulas A, nominals α, and permissions π_1, π_2 such that $\pi_1 \oplus \pi_2$ is defined:*

$$A^{\pi_1 \oplus \pi_2} \models A^{\pi_1} \circledast A^{\pi_2} \tag{Split $\circledast$}$$
$$(\alpha \wedge A)^{\pi_1} \circledast (\alpha \wedge A)^{\pi_2} \models (\alpha \wedge A)^{\pi_1 \oplus \pi_2} \tag{Join $\circledast$}$$

Proof. **Case (Split $\circledast$):** Suppose that $s, h, \rho \models A^{\pi_1 \oplus \pi_2}$. We have $h = (\pi_1 \oplus \pi_2) \cdot h'$, where $s, h', \rho \models A$. That is, for any $\ell \in \mathrm{dom}\,(h)$, we have $h'(\ell) = (v, \pi)$ say and, using the permissions algebra axiom (left-dist) from Definition 3.1,

$$h(\ell) = (v, (\pi_1 \oplus \pi_2) \otimes \pi) = (v, (\pi_1 \otimes \pi) \oplus (\pi_2 \otimes \pi)).$$

Now we define p-heaps h_1 and h_2, both with domain exactly $\mathrm{dom}\,(h)$, by

$$h_i(\ell) = (v, \pi_i \otimes \pi) \;\Leftrightarrow\; h'(\ell) = (v, \pi) \qquad \text{for } i \in \{1, 2\}.$$

By construction, $h_1 = \pi_1 \cdot h'$ and $h_2 = \pi_2 \cdot h'$. Since $s, h', \rho \models A$, this gives us $s, h_1, \rho \models A^{\pi_1}$ and $s, h_2, \rho \models A^{\pi_2}$. Furthermore, also by construction, h_1 and h_2 are compatible, with $h = h_1 \mathbin{\overline{\circ}} h_2$. Thus $s, h, \rho \models A^{\pi_1} \circledast A^{\pi_2}$, as required.

Case (Join $\circledast$): First of all, we show that for any p-heap h,

$$(\pi_1 \cdot h) \mathbin{\overline{\circ}} (\pi_2 \cdot h) = (\pi_1 \oplus \pi_2) \cdot h. \tag{8}$$

To see this, we observe that for any $\ell \in \mathrm{dom}\,(h)$, writing $h(\ell) = (v, \pi)$ say,

$$\begin{aligned}
&((\pi_1 \oplus \pi_2) \cdot h)(\ell) \\
&= (v, (\pi_1 \oplus \pi_2) \otimes \pi) \\
&= (v, (\pi_1 \otimes \pi) \oplus (\pi_2 \otimes \pi)) \qquad \text{by (left-dist)} \\
&= (h_1 \oplus h_2)(\ell) \text{ where } h_1(\ell) = (v, \pi_1 \otimes \pi) \text{ and } h_2 = (v, \pi_2 \otimes \pi) \\
&= ((\pi_1 \cdot h) \mathbin{\overline{\circ}} (\pi_2 \cdot h))(\ell).
\end{aligned}$$

Now, for the main result, suppose $s, h, \rho \models (\alpha \wedge A)^{\pi_1} \circledast (\alpha \wedge A)^{\pi_2}$. We have $h = h_1 \mathbin{\overline{\circ}} h_2$ where $s, h_1, \rho \models (\alpha \wedge A)^{\pi_1}$ and $s, h_2, \rho \models (\alpha \wedge A)^{\pi_2}$. That is, $h = (\pi_1 \cdot h_1') \mathbin{\overline{\circ}} (\pi_2 \cdot h_2')$, where $s, h_1', \rho \models \alpha \wedge A$ and $s, h_2', \rho \models \alpha \wedge A$. Thus $h_1' = h_2' = \rho(\alpha)$ and so, by (8), we have $h = (\pi_1 \oplus \pi_2) \cdot h_1'$, where $s, h_1', \rho \models \alpha \wedge A$. This gives us $s, h, \rho \models (\alpha \wedge A)^{\pi_1 \oplus \pi_2}$, as required.

Lastly, we state some useful principles for labels and the "jump" modality.

Lemma 4.5 (Labelling and jump). *For all formulas A and labels α,*

$$@_\alpha A \wedge \alpha^\pi \models A^\pi \qquad (@\,\text{Elim})$$

$$(\alpha \wedge A)^\pi \models @_\alpha A \qquad (@\,\text{Intro})$$

$$@_\alpha(\beta_1{}^\pi * \beta_2{}^\sigma) \wedge (\beta_1{}^\pi \circledast \beta_2{}^\sigma) \models \alpha \wedge (\beta_1{}^\pi * \beta_2{}^\sigma) \qquad (@/*/\circledast)$$

Proof. We just show the case ($@/*/\circledast$), the others being easy. Suppose $s, h, \rho \models @_\alpha(\beta_1{}^\pi * \beta_2{}^\sigma) \wedge (\beta_1{}^\pi \circledast \beta_2{}^\sigma)$, meaning that $s, \rho(\alpha), \rho \models \beta_1{}^\pi * \beta_2{}^\sigma$ and $s, h, \rho \models \beta_1{}^\pi \circledast \beta_2{}^\sigma$. Then we have $\rho(\alpha) = (\pi \cdot \rho(\beta_1)) \circ (\sigma \cdot \rho(\beta_2))$, while $h = (\pi \cdot \rho(\beta_1)) \mathbin{\overline{\circ}} (\sigma \cdot \rho(\beta_2))$. Since $\circ$ is defined only when its arguments are disjoint p-heaps, we obtain that $h = \rho(\alpha) = (\pi \cdot \rho(\beta_1)) \circ (\sigma \cdot \rho(\beta_2))$. Thus $s, h, \rho \models \alpha \wedge (\beta_1{}^\pi * \beta_2{}^\sigma)$. $\square$

$$\frac{\{A_1\}\,C_1\,\{B_1\} \quad \{A_2\}\,C_2\,\{B_2\}}{\{A_1 \circledast A_2\}\,C_1 \,||\, C_2\,\{B_1 \circledast B_2\}}\ (\boxplus)\ \text{(Par)} \qquad \frac{\{\alpha \wedge A\}\,C\,\{B\}}{\{A\}\,C\,\{B\}}\ (\boxtimes)\ \text{(Label)}$$

$$\frac{\{A\}\,C\,\{B\}}{\{A * F\}\,C\,\{B * F\}}\ (\dagger, \ddagger)\ \text{(Frame } *\text{)} \qquad \frac{\{A\}\,C\,\{B\}}{\{A \circledast F\}\,C\,\{B \circledast F\}}\ (\dagger)\ \text{(Frame } \circledast\text{)}$$

$(\boxplus)\ \mathrm{ModVars}(C_2) \cap \mathrm{FreeVars}(A_1, B_1) = \mathrm{ModVars}(C_1) \cap \mathrm{FreeVars}(A_2, B_2) = \emptyset$
$(\boxtimes)\ \alpha$ fresh $\quad (\dagger)\ \mathrm{ModVars}(C) \cap \mathrm{FreeVars}(F) = \emptyset \quad (\ddagger)$ see §5.3

Fig. 2. The key CSL proof rules used in our examples; not shown are standard rules for consequence, conditionals, load/store, etc. The fresh-labelling rule (Label) and combination of both weak (Frame $\circledast$) and strong (Frame $*$) frame rules are novel to our approach. We require weak conjunction $\circledast$ for the parallel rule (Par).

5 Concurrent Program Verification Examples

In this section, we demonstrate how $\mathsf{SL}_{\mathsf{LP}}$ can be used in conjunction with the usual principles of CSL to construct verification proofs of concurrent programs, taking three examples of increasing complexity.

Our examples all operate on *binary trees* in memory, defined as usual in separation logic (again note the use of $*$ rather than $\circledast$):

$$\mathsf{tree}(x) \ =_{\mathrm{def}}\ (x = \mathit{null} \wedge \mathsf{emp}) \vee (\exists d, l, r.\ x \mapsto (d, l, r) * \mathsf{tree}(l) * \mathsf{tree}(r)).$$

Our proofs employ (a subset of) the standard rules of CSL—with the most important being the concurrency rule from the Introduction, the separation logic *frame rules* for both $*$ and $\circledast$, and a new rule enabling us to introduce fresh labels into the precondition of a triple (similar to the way Hoare logic usually handles existential quantifiers). These key rules are shown in Fig. 2. We simplify our Hoare triple to remove elements to handle function call/return and furthermore omit the presentation of the standard collection of rules for consequence, load, store, if-then-else, assignment, etc.; readers interested in such aspects can consult [1]. Both of our frame rules have the usual side condition on modified program variables. The strong frame rule (Frame $*$) has an additional side condition that will be discussed in Sect. 5.3; until then it is trivially satisfied.

5.1 Parallel Read

Consider the following program:

```
check(x) {
   if (x == null) { return; }
   read(x);  ||  read(x);
}
```

This is intended to be a straightforward example where we take a tree rooted at `x` and, if `x` is non-null, split into parallel threads that run the program `read` on `x`, and whose specification is $\{\alpha^\pi \wedge \mathsf{tree}(x)^\sigma\}$ `read(x)` $\{\alpha^\pi \wedge \mathsf{tree}(x)^\sigma\}$. We prove that `check` satisfies the specification $\{\mathsf{tree}(x)^\pi\}$ `check(x)` $\{\mathsf{tree}(x)^\pi\}$; the verification proof is in Fig. 3. The proof makes use of the basic operations of our theory: labelling, splitting and joining. The example follows precisely these steps, starting by labelling the formula $\mathsf{tree}(x)^\pi \wedge x \neq \mathit{null}$ with α. The concurrency rule (Par) allows us to put formulas back together after the parallel call, and the two copies $(\alpha \wedge \mathsf{tree}(x)^\pi)^{0.5}$ that were obtained are glued back together to yield $\mathsf{tree}(x)^\pi$, since they have the same label.

$\{\mathsf{tree}(x)^\pi\}$
`check(x) {`
$\{(\mathsf{tree}(x)^\pi \wedge x = \mathit{null}) \vee (\mathsf{tree}(x)^\pi \wedge x \neq \mathit{null})\}$
`if (x == null) {` $\{x = \mathit{null} \wedge \mathsf{tree}(x)^\pi\}$
`return;`
$\{\mathsf{tree}(x)^\pi\}$
`}`
$\{\alpha \wedge \mathsf{tree}(x)^\pi \wedge x \neq \mathit{null}\}$ by (Label)
$\{(\alpha \wedge \mathsf{tree}(x)^\pi)^{0.5} \circledast (\alpha \wedge \mathsf{tree}(x)^\pi)^{0.5}\}$ by (Split $\circledast$)

$\{(\alpha \wedge \mathsf{tree}(x)^\pi)^{0.5}\}$	$\|\|$	
$\{\alpha^{0.5} \wedge \mathsf{tree}(x)^{\pi \otimes 0.5}\}$	$\|\|$	by $(\wedge^\pi)$,$(\otimes)$
`read(x);`	$\|\|$	...
$\{\alpha^{0.5} \wedge \mathsf{tree}(x)^{\pi \otimes 0.5}\}$	$\|\|$	
$\{(\alpha \wedge \mathsf{tree}(x)^\pi)^{0.5}\}$	$\|\|$	by $(\wedge^\pi)$,$(\otimes)$

$\{(\alpha \wedge \mathsf{tree}(x)^\pi)^{0.5} \circledast (\alpha \wedge \mathsf{tree}(x)^\pi)^{0.5}\}$ by (Par)
$\{\alpha \wedge \mathsf{tree}(x)^\pi\}$ by (Join $\circledast$)
`}`
$\{\mathsf{tree}(x)^\pi\}$

Fig. 3. Verification proof of program `check` in Example 5.1.

5.2 Parallel Tree Processing (Le and Hobor [24])

Consider the following program, which was also employed as an example in [24]:

```
proc(x) {
   if (x == null) { return; }
   print(x->d);   ||  print(x->d);
   proc(x->l);    ||  proc(x->l);
   proc(x->r);    ||  proc(x->r);
}
```

This code takes a tree rooted at `x` and, if `x` is non-null, splits into parallel threads that call `proc` recursively on its left and right

branches. We prove, in Fig. 4, that `proc` satisfies the specification $\{\alpha \wedge \mathsf{tree}(x)^{\pi}\}\ \texttt{proc(x)}\ \{\alpha \wedge \mathsf{tree}(x)^{\pi}\}$. First we unroll the definition of $\mathsf{tree}(x)$ and distribute the permission over Boolean connectives and $*$. If the tree is empty the process stops. Otherwise, we label each component with a new label and introduce the "jump" statement $@_{\alpha}(\beta_1 * \beta_2 * \beta_3)$, recording the decomposition of the tree into its three components. Since such statements are *pure*, i.e. independent of the heap, we can "carry" this formula along our computation without interfering with the frame rule(s). Now that every subregion is labelled, we split the formula into two copies, each with half share, but after distributing 0.5 over $*$ and $\wedge$ we end up with half shares in the labels as well. We relabel each subregion with new "whole" labels, and again introduce pure @-formulas that record the relation between the old and the new labels. At this moment we enter the parallel threads and recursively apply `proc` to the left and right subtrees of `x`. Assuming the specification of `proc` for subtrees of `x`, we then retrieve the original label α from the trail of crumbs left by the @-formulas. We can then recombine the α-labelled threads using (Join $\circledast$) to arrive at the desired postcondition.

5.3 Cross-thread Data Transfer

Our previous examples involve only "isolated tank" concurrency: a program has some resources and splits them into parallel threads that do not communicate with each other before—remembering Humpty Dumpty!—ultimately re-merging. For our last example, we will show that our technique is expressive enough to handle more sophisticated kinds of sharing, in particular inter-thread coarse-grained communication. We will show that we can not only share read-only data, but in fact prove that one thread has acquired the full ownership of a structure, even when the associated root pointers are not easily exposed.

To do so, we add some communication primitives to our language, together with their associated Hoare rules. Coarse-grained concurrency such as locks, channels, and barriers have been well-investigated in various flavours of concurrent separation logic [19,26,31]. We will use a channel for our example in this section but with simplified rules: the Hoare rule for a channel c to send message number i whose message invariant is R_i^c is $\{R_i^c(x)\}\ \texttt{send}(c, x)\ \{\mathsf{emp}\}$, while the corresponding rule to receive is $\{\mathsf{emp}\}\ \texttt{receive}(c)\ \{\lambda ret.\ R_i^c(ret)\}$. We ignore details such as identifying which party is allowed to send/receive at a given time [14] or the resource ownership of the channel itself [18].

These rules interact poorly with the strong frame rule from Fig. 2:

$$\frac{\{A\}\,C\,\{B\}}{\{A * F\}\,C\,\{B * F\}}\ (\dagger, \ddagger)\ \text{(Frame *)} \qquad \begin{array}{l}(\dagger)\ \mathrm{ModVars}(C) \cap \mathrm{FreeVars}(F) = \emptyset \\ (\ddagger)\ C \text{ does not receive resources}\end{array}$$

The revealed side condition (‡) means that C does not contain any subcommands that "transfer in" resources, such as `unlock`, `receive`, etc.; this side condition is a bit stronger than necessary but has a simple definition and can be checked syntactically. Without (‡), we can reach a contradiction. Assume that the current

$\{\alpha \wedge \mathsf{tree}(x)^{\pi}\}$
`proc(x) {`
$\{(\alpha \wedge (x = null \wedge \mathsf{emp})^{\pi}) \vee (\alpha \wedge (x \mapsto (d,l,r) * \mathsf{tree}(l) * \mathsf{tree}(r))^{\pi})\}$ by $(\wedge^{\pi})$,$(\vee^{\pi})$
$\{(\alpha \wedge x = null \wedge \mathsf{emp}) \vee (\alpha \wedge (x \mapsto (d,l,r) * \mathsf{tree}(l) * \mathsf{tree}(r))^{\pi})\}$
`if (x == null) {` $\{\alpha \wedge x = null \wedge \mathsf{emp}\}$
`return;`
$\{\alpha \wedge (x = null \wedge \mathsf{emp})^{\pi}\}$
$\{\alpha \wedge \mathsf{tree}(x)^{\pi}\}$
`}`
$\{\alpha \wedge (x \overset{\pi}{\mapsto} (d,l,r) * \mathsf{tree}(l)^{\pi} * \mathsf{tree}(r)^{\pi})\}$ by $(*^{\pi})$
$\{((\beta_1 \wedge x \overset{\pi}{\mapsto} (d,l,r)) * (\beta_2 \wedge \mathsf{tree}(l)^{\pi}) * (\beta_3 \wedge \mathsf{tree}(r)^{\pi})) \wedge$ by (Label),
$@_{\alpha}(\beta_1 * \beta_2 * \beta_3)\}$ (@ Intro)
$\{(((\beta_1^{0.5} \wedge x \overset{\pi \otimes 0.5}{\mapsto} (d,l,r)) * (\beta_2^{0.5} \wedge \mathsf{tree}(l)^{\pi \otimes 0.5}) *$
$(\beta_3^{0.5} \wedge \mathsf{tree}(r)^{\pi \otimes 0.5})) \wedge (@_{\alpha}(\beta_1 * \beta_2 * \beta_3))^{0.5}) \circledast$
$(((\beta_1^{0.5} \wedge x \overset{\pi \otimes 0.5}{\mapsto} (d,l,r)) * (\beta_2^{0.5} \wedge \mathsf{tree}(l)^{\pi \otimes 0.5}) *$ by (Split $\circledast$),
$(\beta_3^{0.5} \wedge \mathsf{tree}(r)^{\pi \otimes 0.5})) \wedge (@_{\alpha}(\beta_1 * \beta_2 * \beta_3))^{0.5})\}$ $(*^{\pi})$, $(\wedge^{\pi})$
$\{(((\gamma_1 \wedge x \overset{\pi \otimes 0.5}{\mapsto} (d,l,r) \wedge @_{\gamma_1}\beta_1^{0.5}) * (\gamma_2 \wedge \mathsf{tree}(l)^{\pi \otimes 0.5} \wedge @_{\gamma_2}\beta_2^{0.5}) *$
$(\gamma_3 \wedge \mathsf{tree}(r)^{\pi \otimes 0.5} \wedge @_{\gamma_3}\beta_3^{0.5})) \wedge @_{\alpha}(\beta_1 * \beta_2 * \beta_3)) \circledast$
$(((\gamma_4 \wedge x \overset{\pi \otimes 0.5}{\mapsto} (d,l,r) \wedge @_{\gamma_4}\beta_1^{0.5}) * (\gamma_5 \wedge \mathsf{tree}(l)^{\pi \otimes 0.5} \wedge @_{\gamma_5}\beta_2^{0.5}) *$ by (Label),
$(\gamma_6 \wedge \mathsf{tree}(r)^{\pi \otimes 0.5} \wedge @_{\gamma_6}\beta_3^{0.5})) \wedge @_{\alpha}(\beta_1 * \beta_2 * \beta_3))\}$ (@ Intro)

$\{((\gamma_1 \wedge x \overset{\pi \otimes 0.5}{\mapsto} (d,l,r) \wedge @_{\gamma_1}\beta_1^{0.5}) *$	
$(\gamma_2 \wedge \mathsf{tree}(l)^{\pi \otimes 0.5} \wedge @_{\gamma_2}\beta_2^{0.5}) *$	
$(\gamma_3 \wedge \mathsf{tree}(r)^{\pi \otimes 0.5} \wedge @_{\gamma_3}\beta_3^{0.5})) \wedge @_{\alpha}(\beta_1 * \beta_2 * \beta_3)\}$	
`print(x->d);`	
$\{((\gamma_1 \wedge x \overset{\pi \otimes 0.5}{\mapsto} (d,l,r) \wedge @_{\gamma_1}\beta_1^{0.5}) *$	
$(\gamma_2 \wedge \mathsf{tree}(l)^{\pi \otimes 0.5} \wedge @_{\gamma_2}\beta_2^{0.5}) *$	
$(\gamma_3 \wedge \mathsf{tree}(r)^{\pi \otimes 0.5} \wedge @_{\gamma_3}\beta_3^{0.5})) \wedge @_{\alpha}(\beta_1 * \beta_2 * \beta_3)\}$	
`proc(x->l);`	...
$\{((\gamma_1 \wedge x \overset{\pi \otimes 0.5}{\mapsto} (d,l,r) \wedge @_{\gamma_1}\beta_1^{0.5}) *$	
$(\gamma_2 \wedge \mathsf{tree}(l)^{\pi \otimes 0.5} \wedge @_{\gamma_2}\beta_2^{0.5}) *$	
$(\gamma_3 \wedge \mathsf{tree}(r)^{\pi \otimes 0.5} \wedge @_{\gamma_3}\beta_3^{0.5})) \wedge @_{\alpha}(\beta_1 * \beta_2 * \beta_3)\}$	
`proc(x->r);`	
$\{((\gamma_1 \wedge x \overset{\pi \otimes 0.5}{\mapsto} (d,l,r) \wedge @_{\gamma_1}\beta_1^{0.5}) *$	
$(\gamma_2 \wedge \mathsf{tree}(l)^{\pi \otimes 0.5} \wedge @_{\gamma_2}\beta_2^{0.5}) *$	
$(\gamma_3 \wedge \mathsf{tree}(r)^{\pi \otimes 0.5} \wedge @_{\gamma_3}\beta_3^{0.5})) \wedge @_{\alpha}(\beta_1 * \beta_2 * \beta_3)\}$	
$\{((\beta_1^{0.5} \wedge x \overset{\pi \otimes 0.5}{\mapsto} (d,l,r)) * (\beta_2^{0.5} \wedge \mathsf{tree}(l)^{\pi \otimes 0.5}) *$	
$(\beta_3^{0.5} \wedge \mathsf{tree}(r)^{\pi \otimes 0.5})) \wedge (@_{\alpha}(\beta_1 * \beta_2 * \beta_3))^{0.5}\}$	
$\{(((\beta_1 \wedge x \overset{\pi}{\mapsto} (d,l,r)) * (\beta_2 \wedge \mathsf{tree}(l)^{\pi}) *$	
$(\beta_3 \wedge \mathsf{tree}(r)^{\pi})) \wedge @_{\alpha}(\beta_1 * \beta_2 * \beta_3))^{0.5}\}$	by $(\wedge^{\pi})$,$(*^{\pi})$
$\{(\alpha \wedge (x \overset{\pi}{\mapsto} (d,l,r) * \mathsf{tree}(l)^{\pi} * \mathsf{tree}(r)^{\pi}))^{0.5}\}$	by $(@/*/\circledast)$
$\{(\alpha \wedge (x \overset{\pi}{\mapsto} (d,l,r) * \mathsf{tree}(l)^{\pi} * \mathsf{tree}(r)^{\pi}))^{0.5} \circledast$	
$(\alpha \wedge (x \overset{\pi}{\mapsto} (d,l,r) * \mathsf{tree}(l)^{\pi} * \mathsf{tree}(r)^{\pi}))^{0.5}\}$	by (Par)
$\{\alpha \wedge (x \overset{\pi}{\mapsto} (d,l,r) * \mathsf{tree}(l)^{\pi} * \mathsf{tree}(r)^{\pi})\}$	by (Join $\circledast$)

`}`
$\{\alpha \wedge \mathsf{tree}(x)^{\pi}\}$

Fig. 4. Verification proof of Le and Hobor's program from [24] in Example 5.2.

```
100 void transfer(int key) {   { emp }
101                           rt* = make_tree();
102                           { tree(rt) }
    { (α ∧ tree(rt))^0.5 }                  || { (α ∧ tree(rt))^0.5 }
    tree* sub = find(rt, key)               || ...                          ;
    send(ch, sub)                           || tree* sub = receive(ch)      ;
    ...                                     || modify(sub)                  ;
    receive(ch)                             || send(ch, ())                 ;
    { (ϵ ∧ tree(rt))^0.5 }                  || { (ϵ ∧ tree(rt))^0.5 }
400                           { tree(rt) }
401                           delete_tree(rt);   { emp } }
```

Fig. 5. Verification proof of the top and bottom of `transfer` in Example 5.3.

message invariant R_i^c is $x \overset{0.5}{\mapsto} a$, which has been sent by thread B. Now thread A, which had the other half of $x \overset{0.5}{\mapsto} a$, can reason as follows:

$$\frac{\{\mathsf{emp}\}\ \texttt{receive(c)}\ \{x \overset{0.5}{\mapsto} a\}}{\{\mathsf{emp} * x \overset{0.5}{\mapsto} a\}\ \texttt{receive(c)}\ \{x \overset{0.5}{\mapsto} a * x \overset{0.5}{\mapsto} a\}}\ (\text{Frame } *),\ \text{without } (\ddagger)$$

The postcondition is a contradiction as no location strongly separates from itself. However, given (‡) the strong frame rule can be proven by induction.

The consequence of (‡), from a verification point of view, is that when resources are transferred in they arrive *weakly separated*, by ⊛, since we must use the weak frame rule around the receiving command. The troublesome issue is that this newly "arriving" state can thus ⊛-overlap awkwardly with the existing state. Fortunately, judicious use of labels can sort things out.

Consider the code in Fig. 5. The basic idea is simple: we create some data at the top (line 101) and then split its ownership 50-50 to two threads. The left thread finds a subtree, and passes its half of that subtree to the right via a channel. The right thread receives the root of that subtree, and thus has full ownership of that subtree along with half-ownership of the rest of the tree. Accordingly, the right thread can modify that subtree before notifying the left subtree and passing half of the modified subtree back. After merging, full ownership of the entire tree is restored and so on line 401 the program can delete it. Figure 5 only contains the proof and line numbers for the top and bottom shared portions. The left and the right thread's proofs appear in Fig. 6.

By this point the top and bottom portions of the verification are straightforward. After creating the tree $\mathsf{tree}(rt)$ at line 102, we introduce the label α, split the formula using (Split ⊛), and then pass $(\alpha \wedge \mathsf{tree}(rt))^{0.5}$ to both threads. After the parallel execution, due to the call to `modify(sub)` in the right thread, the tree has changed in memory. Accordingly, the label for the tree must also change as indicated by the $(\epsilon \wedge \mathsf{tree}(rt))^{0.5}$ in both threads after parallel processing. These are then recombined on line 400 using the re-combination principle (Join ⊛), before the tree is deallocated via standard sequential techniques.

200 $\{\ (\alpha \wedge \mathsf{tree}(\mathtt{rt}))^{0.5}\ \}$
201 `tree* sub = find(rt, key);`
202 $\{\ \left(\alpha^{0.5} \wedge \mathsf{tree}(\mathtt{sub}) * (\mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \mathsf{tree}(\mathtt{rt}))\right)^{0.5}\ \}$
203 $\{\ \left(\alpha^{0.5} \wedge (\beta \wedge \mathsf{tree}(\mathtt{sub})) * (\gamma \wedge (\mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \mathsf{tree}(\mathtt{rt})))\right)^{0.5}\ \}$
204 $\left\{\begin{array}{l} \alpha^{0.5} \wedge \left((\beta \wedge \mathsf{tree}(\mathtt{sub})) * (\gamma \wedge (\mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \mathsf{tree}(\mathtt{rt})))\right)^{0.5} \wedge \\ \left(@_\alpha^{0.5}((\beta \wedge \mathsf{tree}(\mathtt{sub})) * (\gamma \wedge (\mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \mathsf{tree}(\mathtt{rt}))))^{0.5}\right) \end{array}\right\}$
205 $\left\{\begin{array}{l} (\beta \wedge \mathsf{tree}(\mathtt{sub}))^{0.5} * (\gamma \wedge (\mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \mathsf{tree}(\mathtt{rt})))^{0.5} \wedge \\ \left(@_\alpha^{0.5}((\beta \wedge \mathsf{tree}(\mathtt{sub})) * (\gamma \wedge (\mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \mathsf{tree}(\mathtt{rt}))))^{0.5}\right) \end{array}\right\}$
206 $\left\{\begin{array}{l} (\gamma \wedge (\mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \mathsf{tree}(\mathtt{rt})))^{0.5} \circledast (\beta \wedge \mathsf{tree}(\mathtt{sub}))^{0.5} \wedge \\ \left(@_\alpha^{0.5}((\beta \wedge \mathsf{tree}(\mathtt{sub})) * (\gamma \wedge (\mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \mathsf{tree}(\mathtt{rt}))))^{0.5}\right) \end{array}\right\}$
207 `send(ch, sub);`
208 $\{\ (\gamma \wedge (\mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \mathsf{tree}(\mathtt{rt})))^{0.5}\ \}$
209 `...`
210 $\{\ (\gamma \wedge (\mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \mathsf{tree}(\mathtt{rt})))^{0.5}\ \}$
211 `receive(ch);`
212 $\left\{\begin{array}{l} (\gamma \wedge (\mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \mathsf{tree}(\mathtt{rt})))^{0.5} \circledast \left((@_\gamma^{0.5}(\delta \wedge \mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \epsilon \wedge \mathsf{tree}(\mathtt{rt}))^{0.5}) \wedge \right. \\ \left. \gamma \perp \delta \wedge \delta \wedge \mathsf{tree}(\mathtt{sub})^{0.5}\right) \end{array}\right\}$
213 $\{\ \gamma \wedge (\delta \wedge \mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \epsilon \wedge \mathsf{tree}(\mathtt{rt}))^{0.5} \circledast \delta \wedge \mathsf{tree}(\mathtt{sub})^{0.5} \wedge \ \gamma \perp \delta\}$
214 $\{\ (\delta \wedge \mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \epsilon \wedge \mathsf{tree}(\mathtt{rt}))^{0.5} * \delta \wedge \mathsf{tree}(\mathtt{sub})^{0.5}\ \}$
215 $\{\ (\epsilon \wedge \mathsf{tree}(\mathtt{rt}))^{0.5}\ \}$

---

300 $\{\ (\alpha \wedge \mathsf{tree}(\mathtt{rt}))^{0.5}\ \}$
301 `...`
302 $\{\ (\alpha \wedge \mathsf{tree}(\mathtt{rt}))^{0.5}\ \}$
303 `tree* sub = receive(ch);`
304 $\left\{\begin{array}{l} (\alpha \wedge \mathsf{tree}(\mathtt{rt}))^{0.5} \circledast (\beta \wedge \mathsf{tree}(\mathtt{sub}))^{0.5} \wedge \\ \left(@_\alpha^{0.5}((\beta \wedge \mathsf{tree}(\mathtt{sub})) * (\gamma \wedge (\mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \mathsf{tree}(\mathtt{rt}))))^{0.5}\right) \end{array}\right\}$
305 $\{\ ((\beta \wedge \mathsf{tree}(\mathtt{sub})) * (\gamma \wedge (\mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \mathsf{tree}(\mathtt{rt}))))^{0.5} \circledast (\beta \wedge \mathsf{tree}(\mathtt{sub}))^{0.5}\ \}$
306 $\{\ ((\beta \wedge \mathsf{tree}(\mathtt{sub}))^{0.5} \circledast (\beta \wedge \mathsf{tree}(\mathtt{sub}))^{0.5}) * (\gamma \wedge (\mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \mathsf{tree}(\mathtt{rt})))^{0.5}\ \}$
307 $\{\ \mathsf{tree}(\mathtt{sub}) * (\gamma \wedge (\mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \mathsf{tree}(\mathtt{rt})))^{0.5}\ \}$
308 `modify(sub);`
309 $\{\ \mathsf{tree}(\mathtt{sub}) * (\gamma \wedge (\mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \mathsf{tree}(\mathtt{rt})))^{0.5}\ \}$
310 $\{\ (\delta \wedge \mathsf{tree}(\mathtt{sub})) * (\gamma \wedge ((\delta \wedge \mathsf{tree}(\mathtt{sub})) \mathrel{-\!\!*} (\epsilon \wedge \mathsf{tree}(\mathtt{rt}))))^{0.5} \wedge \gamma \perp \delta\ \}$
311 $\left\{\begin{array}{l} ((\delta \wedge \mathsf{tree}(\mathtt{sub}))^{0.5} \circledast (\delta \wedge \mathsf{tree}(\mathtt{sub}))^{0.5}) * (\gamma \wedge ((\delta \wedge \mathsf{tree}(\mathtt{sub})) \mathrel{-\!\!*} (\epsilon \wedge \mathsf{tree}(\mathtt{rt}))))^{0.5} \wedge \\ \gamma \perp \delta \wedge \left(@_\gamma^{0.5}((\delta \wedge \mathsf{tree}(\mathtt{sub})) \mathrel{-\!\!*} (\epsilon \wedge \mathsf{tree}(\mathtt{rt})))^{0.5}\right) \end{array}\right\}$
312 $\left\{\begin{array}{l} ((\delta \wedge \mathsf{tree}(\mathtt{sub}))^{0.5} * (\gamma \wedge ((\delta \wedge \mathsf{tree}(\mathtt{sub})) \mathrel{-\!\!*} (\epsilon \wedge \mathsf{tree}(\mathtt{rt}))))^{0.5}) \circledast \\ (\delta \wedge \mathsf{tree}(\mathtt{sub}))^{0.5} \wedge \gamma \perp \delta \wedge \left(@_\gamma^{0.5}((\delta \wedge \mathsf{tree}(\mathtt{sub})) \mathrel{-\!\!*} (\epsilon \wedge \mathsf{tree}(\mathtt{rt})))^{0.5}\right) \end{array}\right\}$
313 $\left\{\begin{array}{l} (\epsilon \wedge \mathsf{tree}(\mathtt{rt}))^{0.5} \circledast \\ (\delta \wedge \mathsf{tree}(\mathtt{sub}))^{0.5} \wedge \gamma \perp \delta \wedge \left(@_\gamma^{0.5}((\delta \wedge \mathsf{tree}(\mathtt{sub})) \mathrel{-\!\!*} (\epsilon \wedge \mathsf{tree}(\mathtt{rt})))^{0.5}\right) \end{array}\right\}$
314 `send(ch, ());`
315 $\{\ (\epsilon \wedge \mathsf{tree}(\mathtt{rt}))^{0.5}\ \}$

Fig. 6. Verifications of the left (top) and right (bottom) threads of `transfer`.

Let us now examine the more interesting proofs of the individual threads in Fig. 6. Line 201 calls the `find` function, which searches a binary tree for a subtree rooted with key `key`. Following Cao *et al.* [13] we specify `find` as follows:

$$\{\ \mathsf{tree}(x)^\pi\ \}\ \mathtt{find}(x)\ \{\ \lambda ret.\ \left(\mathsf{tree}(ret) * (\mathsf{tree}(ret) \mathrel{-\!\!*} \mathsf{tree}(x))\right)^\pi\ \}$$

Here *ret* is bound to the return value of `find`, and the postcondition can be considered to represent the returned subtree $\mathsf{tree}(ret)$ separately from the tree-with-a-hole $\mathsf{tree}(ret) \mathrel{-\!\!*} \mathsf{tree}(x)$, using a $*/\mathrel{-\!\!*}$ style to represent replacement as per Hobor and Villard [20]. This is the invariant on line 202.

Line 203 then attaches the fresh labels β and γ to the $*$-separated subparts, and line 204 snapshots the formula current at label α using the @ operator; $@^{\pi}_{\alpha} P$ should be read as "when one has a π-fraction of α, P holds"; it is definable using @ and an existential quantifier over labels. On line 205 we forget (in the left thread) the label α for the current heap for housekeeping purposes, and then on line 206 we weaken the strong separating conjunction $*$ to the weak one $\circledast$ before sending the root of the subtree `sub` on line 207.

In the `transfer` program, the invariant for the first channel message is

$$(\beta \wedge \mathsf{tree}(\mathtt{sub}))^{0.5} \wedge \left(@^{0.5}_{\alpha}((\beta \wedge \mathsf{tree}(\mathtt{sub})) * (\gamma \wedge (\mathsf{tree}(\mathtt{sub}) \mathrel{-\!\!*} \mathsf{tree}(\mathtt{rt}))))^{0.5}\right)$$

In other words, half of the ownership of the tree rooted at `sub` plus the (pure) @-fact about the shape of the heap labeled by α. Comparing lines 206 and 208 we can see that this information has been shipped over the wire (the @-information has been dropped since no longer needed). The left thread then continues to process until synchronizing again with the `receive` in line 211.

Before we consider the second synchronization, however, let us instead jump to the corresponding receive in the right thread at line 303. After the receive, the invariant on line 304 has the (weakly separated) resources sent from the left thread on line 206. We then "jump" label α using the @-information to reach line 305. We can redistribute the β inside the $*$ on line 306 since we already know that β and γ are disjoint. On line 307 we reach the payoff by combining both halves of the subtree `sub`, enabling the modification of the subtree in line 308.

On line 310 we label the two subheaps, and specialize the magic wand so that given the specific heap δ it will yield the specific heap ϵ; we also record the pure fact that γ and δ are disjoint, written $\gamma \perp \delta$. On line 311 we snapshot γ and split the tree `sub` 50-50; then on line 312 we push half of `sub` out of the strong $*$. On line 313 we combine the subtree and the tree-with-hole to reach the final tree ϵ. We then send on line 314 with the channel's second resource invariant:

$$(\delta \wedge \mathsf{tree}(\mathtt{sub}))^{0.5} \wedge \gamma \perp \delta \wedge \left(@^{0.5}_{\gamma}((\delta \wedge \mathsf{tree}(\mathtt{sub})) \mathrel{-\!\!*} (\epsilon \wedge \mathsf{tree}(\mathtt{rt})))^{0.5}\right)$$

After the send, on line 315 we have reached the final fractional tree ϵ.

Back in the left-hand thread, the second send is received in line 211, leading to the weakly-separated postcondition in line 212. In line 213 we "jump" label γ, and then in line 214 we use the known disjointness of γ and δ to change the $\circledast$ to $*$. Finally in line 215 we apply the magic wand to reach the postcondition.

6 Conclusions and Future Work

We propose an extension of separation logic with fractional permissions [4] in order to reason about sharing over arbitrary regions of memory. We identify two

fundamental logical principles that fail when the "weak" separating conjunction $\circledast$ is used in place of the usual "strong" $*$, the first being distribution of permissions—$A^\pi \circledast B^\pi \not\models (A \circledast B)^\pi$—and the second being the re-combination of permission-divided formulas, $A^\pi \circledast A^\sigma \not\models A^{\pi \oplus \sigma}$. We avoid the former difficulty by *retaining* the strong $*$ in the formalism alongside $\circledast$, and the latter by using nominal *labels*, from hybrid logic, to record exact aliasing between read-only copies of a formula.

The main previous work addressing these issues, by Le and Hobor [24], uses a combination of permissions based on *tree shares* [17] and semantic side conditions on formulas to overcome the aforementioned problems. The *rely-guarantee* separation logic in [30] similarly restricts concurrent reasoning to structures described by precise formulas only. In contrast, our logic is a little more complex, but we can use permissions of any kind, and do not require side conditions. In addition, our use of labelling enables us to handle examples involving the transfer of data structures between concurrent threads.

On the other hand, we think it probable that the kind of examples we consider in this paper could also be proven by hand in at least some of the verification formalisms derived from CSL (e.g. [16,22,27]). For example, using the "concurrent abstract predicates" in [16], one can explicitly declare shared regions of memory in a fairly ad-hoc way. However, such program logics are typically very complicated and, we believe, quite unlikely to be amenable to automation.

We feel that the main appeal of the present work lies in its relative simplicity—we build on standard CSL with permissions and invoke only a modest amount of extra syntax—which bodes well for its potential automation (at least for simpler examples). In practical terms, an obvious way to proceed would be to develop a prototype verifier for concurrent programs based on our logic $\mathsf{SL}_{\mathsf{LP}}$. An important challenge in this area is to develop heuristics—e.g., for splitting, labelling and combining formulas—that work acceptably well in practice.

An even greater challenge is to move from *verifying* user-provided specifications to *inferring* them automatically, as is done e.g. by Facebook Infer. In separation logic, this crucially depends on solving the *biabduction* problem, which aims to discover "best fit" solutions for applications of the frame rule [9,11]. In the CSL setting, a further problem seems to lie in deciding how applications of the concurrency rule should divide resources between threads.

Finally, automating the verification approach set out in this paper will likely necessitate restricting our full logic to some suitably tractable fragment, e.g. one analogous to the well-known *symbolic heaps* in standard separation logic (cf. [2,15]). The identification of such tractable fragments is another important theoretical problem in this area. It is our hope that this paper will serve to stimulate interest in the automation of concurrent separation logic in particular, and permission-sensitive reasoning in general.

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Local Reasoning About the Presence of Bugs: Incorrectness Separation Logic

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Abstract. There has been a large body of work on local reasoning for proving the *absence* of bugs, but none for proving their *presence*. We present a new formal framework for local reasoning about the presence of bugs, building on two complementary foundations: 1) separation logic and 2) incorrectness logic. We explore the theory of this new *incorrectness separation logic* (ISL), and use it to derive a begin-anywhere, intra-procedural symbolic execution analysis that has no false positives *by construction*. In so doing, we take a step towards transferring modular, scalable techniques from the world of program verification to bug catching.

Keywords: Program logics · Separation logic · Bug catching

1 Introduction

There has been significant research on sound, local reasoning about the state for proving the absence of bugs (e.g., [2,13,26,29,30,41]). Locality leads to techniques that are compositional *both* in code (concentrating on a program component) and in the resources accessed (spatial locality), without tracking the entire global state or the global program within which a component sits. Compositionality enables reasoning to scale to large teams and codebases: reasoning can be done even when a global program is not present (e.g., a library, or during program construction), without having to write the analogue of a test or verification harness, and the results of reasoning about components can be composed efficiently [11].

Meanwhile, many of the practical applications of symbolic reasoning have aimed at proving the *presence* of bugs (i.e., bug catching), rather than proving their absence (i.e., correctness). Logical bug catching methods include symbolic model checking [7,12] and symbolic execution for testing [9]. These methods are usually formulated as global analyses; but, the rationale of local reasoning holds just as well for bug catching as it does for correctness: it has the potential to

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benefit scalability, reasoning about incomplete code, and continuous incremental reasoning about a changing codebase within a continuous integration (CI) system [34]. Moreover, local evidence of a bug without usually-irrelevant contextual information can be more convincing and easier to understand and correct.

There do exist symbolic bug catchers that, at least partly, address scalability and continuous reasoning. Tools such as Coverity [5,32] and Infer [18] hunt for bugs in large codebases with tens of millions of LOC, and they can even run incrementally (within minutes for small code changes), which is compatible with deployment in CI to detect regressions. However, although such tools intuitively share ideas with correctness-based compositional analyses [16], the existing foundations of correctness-based analyses do not adequately explain what these bug-catchers do, why they work, or the extent to which they work in practice.

A notable such example is the relation between *separation logic* (SL) and Infer. SL provides novel techniques for local reasoning [28], with concise specifications that focus only on the memory accessed [36]. Using SL, symbolic execution need not begin from a "main" program, but rather can "begin anywhere" in a codebase, with constraints on the environment synthesized along the way. When analyzing a component, SL's frame rule is used in concert with abductive inference to isolate a description of the memory utilized by the component [11]. Infer was closely inspired by SL, and demonstrates the power of SL's local reasoning: the ability to begin anywhere supports incremental analysis in CI, and compositionality leads to highly scalable methods. These features have led to non-trivial impact: a recent paper quotes over 100,000 Infer-reported bugs fixed in Facebook's codebases, and thousands of security bugs found by a compositional taint analyzer, Zoncolan [18]. However, Infer reports bugs using *heuristics based on failed proofs*, whereas the SL theory behind Infer is based on *over-approximation* [11]. Thus, a critical aspect of Infer's successful deployment is not supported by the theory that inspired it. This is unfortunate, especially given that the begin-anywhere and scalable aspects of Infer's algorithms do not appear to be fundamentally tied to over-approximation.

In this paper, we take a step towards transferring the local reasoning techniques from the world of program verification to that of bug catching. To approach the problem from first principles, we do not try to understand tools such as Coverity and Infer as they are. Instead, we take their existence and reported impact as motivation for revisiting the foundations of SL, this time re-casting it as a formalism for proving the *presence* of bugs rather than their absence.

Our new logic, *incorrectness separation logic* (ISL), marries local reasoning based on SL's frame rule with the recently-advanced incorrectness logic [35], a formalism for reasoning about errors based on an *under-approximate* analogue of Hoare triples [43]. We observe that the original SL model, based on partial heaps, is incompatible with local, under-approximate reasoning. The problem is that the original model does not distinguish a pointer known to be dangling from one about which we have no knowledge; this in turn contradicts the frame rule for under-approximate reasoning. However, we recover the frame rule for a

refined model with negative heap assertions of the form $x \not\mapsto$, read "invalidated x", stating that the location at x has been deallocated (and not re-allocated). Negative heaps were present informally in the original Infer, unsupported by theory but added for reporting use-after-free bugs (i.e., not for proving correctness). Interestingly, this semantic feature is needed in ISL for logical (and not merely pragmatic) reasons, in that it yields a *sound* logic for proving the presence of bugs: when ISL identifies a bug, then there is indeed a bug (no false positives), given the assumptions of the underlying ISL model. (That is, as usual, soundness is a relationship between assumptions and conclusions, and whether those assumptions match reality (i.e., running code) is a separate concern, outside the purview of logic.)

As well as being superior for bug reporting, our new model has a pleasant fundamental property in that it meshes better with intuitions originally expressed of SL. Specifically, our model admits a *footprint theorem*, stating that the meaning of a command is solely determined by its transitions on input-output heaplets of minimal size (including only the locations accessed), a theorem that was not true in full generality for the original SL model. Interestingly, ISL supports local reasoning for technically simpler reasons than the original SL (see Sect. 4.2).

We validate part of the ISL promise using an illustrative program analysis, Pulse, and use it to detect *memory safety bugs*, namely null-pointer-dereference and use-after-free bugs. Pulse is written inside Infer [18] and deployed at Facebook where it is used to report issues to C++ developers. Pulse is currently under active development. In this paper, we explore the *intra-procedural* analysis, i.e., how it provides purely local reasoning about one procedure at a time without using results from other procedures; we defer formalising its *inter-procedural* (between procedures) analysis to future work. While leaving out the inter-procedural capabilities of Pulse only partly validates the promise of the ISL theory, it already demonstrates how ISL can scale to large codebases, and run incrementally in a way compatible with CI. Pulse thus has the capability to begin anywhere, and it achieves scalability while embracing under- rather than over-approximation.

Outline. In Sect. 2 we present an intuitive account of ISL. In Sect. 3 we present the ISL proof system. In Sect. 4 we present the semantic model of ISL. In Sect. 5 we present our ISL-based Pulse analysis. In Sect. 6 we discuss related work and conclude. The full proofs of all stated theorems are given in the technical appendix [38].

2 Proof of a Bug

We proceed with an intuitive description of ISL for detecting memory safety bugs. To do this, in Fig. 1 we present an example of C++ use-after-lifetime bug, abstracted from real occurrences we have observed at Facebook, where use-after-lifetime bugs were one of the leading developer requests for C++ analysis. Given a vector `v`, a call to `push_back(v)` in the `std::vector` library may cause the internal array backing `v` to be (deallocated and subsequently) reallocated when `v`

```
void deref_after_pb(std::vector<int> *v) {
  int *x = &v->at(1);
  v->push_back(42);
  std::cout << *x << "\n"; }
```

```
push_back.cpp:7: error: VECTOR_INVALIDATION. accessing memory that was
potentially invalidated by 'std::vector::push_back()'  on line 6.
  5.     int *x = &(v->at(1));
  6.     v->push_back(42);
  7. >   std::cout << *x << "\n"; }
```

Fig. 1. The C++ use-after-lifetime bug (above); the Pulse error message (below).

needs to grow to accommodate new elements. If the internal array is reallocated during the `v->push_back(42)` call, a use-after-lifetime bug occurs on the next line as `x` points into the previous array. Note how the Pulse error message (at the bottom of Fig. 1) refers to memory that has been invalidated. As we describe shortly, this information is tracked in Pulse with an invalidated heap assertion.

For the theory in this paper, we do not want to descend into the details of C++, vectors, and so forth. Thus, for illustrative purposes, in Fig. 2 we present an adaptation of such use-after-lifetime bugs in C rather than C++, alongside its representation in the ISL language used in this paper. In this adaptation, the array at v is of size 1, and is reallocated in `push_back` non-deterministically to model its dynamic reallocation when growing. We next demonstrate how we can use ISL to detect the use-after-lifetime bug in the `client` procedure in Fig. 2.

ISL Triples. The ISL theory uses *under-approximate triples* [35] of the form [presumption] $\mathbb{C}$ [ϵ : result], interpreted as: the result assertion describes a *subset* of the states that can be reached from the presumption assertion by executing $\mathbb{C}$, where ϵ denotes an *exit condition* indicating either normal or exceptional (erroneous) termination. The under-approximate triples can be equivalently interpreted as: every state in result can be obtained by executing $\mathbb{C}$ on a starting state in presumption. By contrast, given a Hoare triple {pre} $\mathbb{C}$ {post}, the post-condition post describes a *superset* of states that are reachable from the pre-condition pre, and may include states unreachable from pre. Hoare logic is about over-approximation, allowing false positives but not negatives, whereas ISL is about under-approximation, allowing false negatives but not positives.

Bug Specification of `client(`v`)`. Using ISL, we can specify the use-after-lifetime bug in `client(`v`)` as follows:

$$[v \mapsto a * a \mapsto -] \texttt{ client(}v\texttt{)} \ [er(\mathrm{L}_{rx}) : \exists a'.\ v \mapsto a' * a' \mapsto - * a \not\mapsto] \qquad \text{(PB-Client)}$$

We make several remarks to illustrate the crucial features of ISL:

- As in standard SL, $*$ denotes the separating conjunction, read "and separately". It implies, e.g., that v, a' and a are distinct in the result assertion.
- The exit condition $er(\mathrm{L}_{rx})$ denotes an erroneous termination: an error state is reached at line L_{rx}, where a is dangling (invalidated).

```
void push_back(int **v)
{
  if (nondet()) {
    free(*v);
    *v = malloc(sizeof(int));
  }
}

void client(v) {
  int* x = *v;
  push_back(v);
  *x = 88; }
```

```
push_back(v) ≜
  local z, y in
      z := *;
      (assume(z ≠ 0); L_rv: y := [v];
       L_f: free(y);
       y := malloc(); [v] := y)
    + (assume(z = 0); skip)

client(v) ≜
  local x in
    x := [v];
    push_back(v);
    L_rx: [x] := 88
```

Fig. 2. The `push_back` example in C (left); and in the ISL language (right).

- The result is under-approximate: any state satisfying the result assertion can be reached from some state satisfying the presumption.
- The specification is local: it focuses only on memory locations in the `client(`v`)` footprint (i.e., those touched by `client(`v`)`), and ignores other locations.

Let us next consider how we reason symbolically about this bug. Note that for the `client(`v`)` execution to reach an error at line L_{rx}, the `push_back(`v`)` call within it must not cause an error. That is, in contrast to PB-Client, we need a specification for `push_back(`v`)` that describes normal, non-erroneous termination. We specify this normal execution with the *ok* exit condition as follows:

$$[v \mapsto a * a \mapsto -]\ \texttt{push\_back}(v)\ [ok : \exists a'.\ v \mapsto a' * a' \mapsto - * a \not\mapsto]\quad \text{(PB-Ok)}$$

PB-Ok describes the case when `push_back(`v`)` frees the internal array of v at a (denoted by $a \not\mapsto$ in the result), and subsequently reallocates it at a'. Consequently, as a is invalidated after the `push_back(`v`)` call, the instruction following the call in `client(`v`)` dereferences invalidated memory at L_{rx}, causing an error.

Note that the result assertion in PB-Ok is strictly under-approximate in that it is smaller (stronger) than the exact "strongest post". Given the assertion in the presumption, the strongest post must also consider the else clause of the conditional, when `nondet()` returns zero and `push_back(`v`)` does nothing. That is, the strongest post is the disjunction of the given result and the presumption. The ability to go below the strongest post soundly is a hallmark of under-approximate reasoning: it allows for compromise in an analyzer, where we might choose, e.g., to limit the number of paths explored for efficiency reasons, or to concretize an assertion partially when symbolic reasoning becomes difficult [35].

We present proof outlines for PB-Ok and PB-Client in Fig. 3, where we annotate each step with a proof rule to connect to the ISL theory in Sect. 3. For

legibility, uses of the FRAME rule are omitted as it is used in almost every step, and the consequence rule CONS is usually omitted when rewriting a formula to an equivalent one. For the moment, we encourage the reader to attempt to follow, prior to formalization, by mentally executing the program instructions on the assertions and asking: does the assertion at each program point under-approximate the states that can be obtained from the prior state? Note that each step updates assertions in-place, just as concrete execution does on concrete memory. For example, L_f: `free(`y`)` replaces $a \mapsto -$ with $a \not\mapsto$. In-place reasoning is a capability that the separating conjunction brings to symbolic execution; formally, this in-place aspect is achieved in the logic by applying the frame rule.

3 Incorrectness Separation Logic (ISL)

As a first attempt, it is tempting to obtain ISL straightforwardly by composing the standard semantics of SL [41] and the semantics of incorrectness logic [35]. Interestingly, this simplistic approach does not work. To see this, consider the following axiom for freeing memory, adapted from the corresponding SL axiom:

$$[x \mapsto -]\ \texttt{free}(x)\ [ok\colon \texttt{emp} \wedge \texttt{loc}(x)]$$

Here, `emp` describes the empty heap and `loc`(x) states that x is an addressable location; e.g., x cannot be `null`. Note that this ISL triple is valid in that any state satisfying the result assertion can be obtained from one satisfying the presumption assertion, and thus we do have a true under-approximate triple.

However, in SL one can arbitrarily extend the state using the frame rule:

$$\frac{\vdash [p]\ \mathbb{C}\ [\epsilon : q] \qquad \mathsf{mod}(\mathbb{C}) \cap \mathsf{fv}(r) = \emptyset}{\vdash [p * r]\ \mathbb{C}\ [\epsilon : q * r]}\ (\textsc{Frame})$$

Intuitively, the state described by the *frame* assertion r lies outside the footprint of $\mathbb{C}$ and thus remains unchanged when executing $\mathbb{C}$. However, if we do this with the `free`(x) axiom above, choosing $x \mapsto -$ as our frame, we run into a problem:

$$[x \mapsto - * x \mapsto -]\ \texttt{free}(x)\ [ok\colon (\texttt{emp} \wedge \texttt{loc}(x)) * x \mapsto -]$$

Here, the presumption is inconsistent but the result is not, and thus there is no way to get back to the presumption from the result; i.e., the triple is invalid. In over-approximate reasoning this does not cause a problem since an inconsistent precondition renders an over-approximate triple vacuously valid. By contrast, an inconsistent presumption does not validate under-approximate reasoning.

Our way out of this conundrum is to consider a modified model in which the knowledge that a location was previously freed is a resource-oriented fact, using negative heap assertions. The negative heap assertion $x \not\mapsto$ conveys more knowledge than the `loc`(x) assertion. Specifically, $x \not\mapsto$ conveys: 1) the *knowledge* that x is an addressable location; 2) the knowledge that x has been deallocated; and 3) the *ownership* of location x. In other words, $x \not\mapsto$ is analogous to the

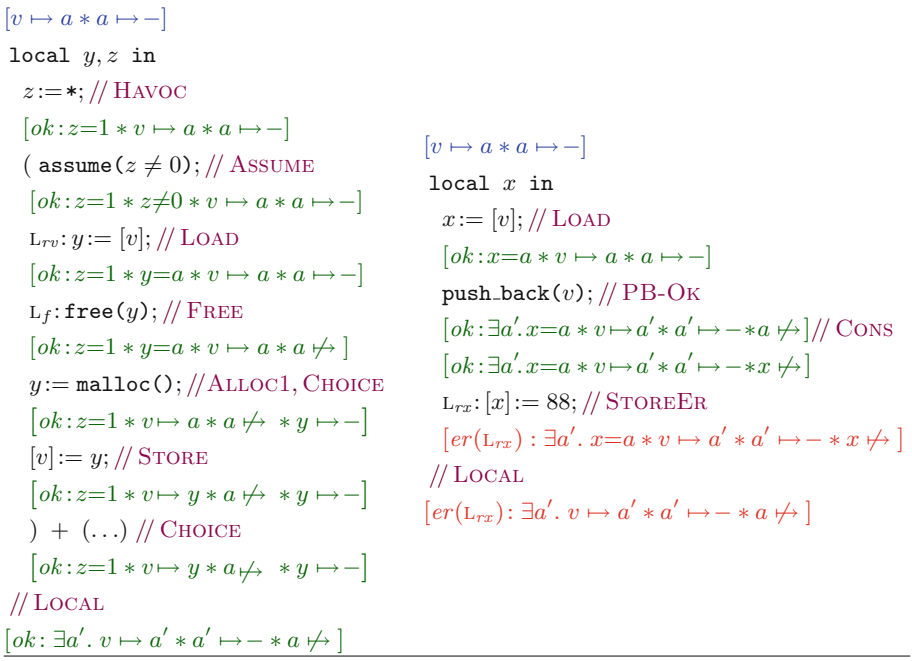

Fig. 3. The proof sketches of PB-OK (left) and PB-CLIENT (right).

points-to assertion $x \mapsto -$ and is thus manipulated similarly, taking up space in $*$-conjuncts. That is, we cannot consistently $*$-conjoin $x \not\mapsto$ either with $x \mapsto -$ or with itself: $x \mapsto - * x \not\mapsto \Leftrightarrow \mathsf{false}$ and $x \not\mapsto * x \not\mapsto \Leftrightarrow \mathsf{false}$.

With such negative assertions, we can specify `free()` as the FREE axiom in Fig. 5. Note that this allows us to recover the frame rule: when we frame $x \mapsto -$ on both sides, we obtain the inconsistent assertion $x \mapsto - * x \not\mapsto$ (i.e., false) in the result, which always makes an under-approximate triple vacuously valid.

We demonstrated how we arrived at negative heaps as a theoretical solution to recover the frame rule. However, negative heaps are more than a technical curiosity. In particular, a similar idea was informally present in Infer and has been used formally to reason about JavaScript [21]. Moreover, as we show in Sect. 4, negative heaps give rise to a *footprint theorem* (see Theorem 2).

Negative heap assertions were previously used informally in Infer. They were also independently and formally introduced in a separation logic for JavaScript [21] to state that a field is not present in a JavaScript object, which is a natural property to express when reasoning about JavaScript.

$$\textsc{Comm} \ni \mathbb{C} ::= \texttt{skip} \mid x := e \mid x := \texttt{*} \mid \texttt{assume}(B) \mid \texttt{local}\ x\ \texttt{in}\ \mathbb{C} \mid \mathbb{C}_1; \mathbb{C}_2 \mid \mathbb{C}_1 + \mathbb{C}_2 \mid \mathbb{C}^\star \mid x := \texttt{alloc}() \mid \textsc{l}\colon \texttt{free}(x) \mid \textsc{l}\colon x := [y] \mid \textsc{l}\colon [x] := y \mid \textsc{l}\colon \texttt{error}$$

$$\begin{aligned} \texttt{if}\ B\ \texttt{then}\ \mathbb{C}_1\ \texttt{else}\ \mathbb{C}_2 &\triangleq (\texttt{assume}(B); \mathbb{C}_1) + (\texttt{assume}(!B); \mathbb{C}_2) \\ \texttt{while}(B)\ \mathbb{C} &\triangleq (\texttt{assume}(B); \mathbb{C})^\star; \texttt{assume}(!B) \\ \texttt{assert}(B) &\triangleq (\texttt{assume}(!B); \texttt{error}) + \texttt{assume}(B) \\ x := \texttt{malloc}() &\triangleq x := \texttt{alloc}() \ + \ x := \texttt{null} \end{aligned}$$

Fig. 4. The ISL Language (above); encoding standard constructs in ISL (below).

Programming Language. To keep our presentation concise, we employ a simple heap-manipulating language as shown in Fig. 4. We assume an infinite set Val of *values*; a finite set Var of (program) *variables*; a standard interpreted language for *expressions*, Exp, containing variables and values; and a standard interpreted language for *Boolean expressions*, BExp. We use v as a metavariable for values; x, y, z for program variables; e for expressions; and B for Boolean expressions.

Our language is given by the $\mathbb{C}$ grammar and includes the standard constructs of `skip`, assignment ($x := e$), non-deterministic assignment ($x :=$ `*`, where `*` denotes a non-deterministically picked value), assume statements (`assume(`B`)`), scoped variable declaration (`local` x `in` $\mathbb{C}$), sequential composition ($\mathbb{C}_1; \mathbb{C}_2$), non-deterministic choice ($\mathbb{C}_1 + \mathbb{C}_2$) and loops ($\mathbb{C}^\star$), as well as error statements (`error`) and heap-manipulating instructions. Note that deterministic choice and loops (e.g.,`if` and `while` statements) can be encoded using their non-deterministic counterparts and assume statements, as shown in Fig. 4.

To better track errors, we annotate instructions that may cause an error with a label $\textsc{l} \in \textsc{Label}$. When an error is encountered (e.g., in $\textsc{l}\colon$ `error`), we report the label of the offending instruction (e.g., l). As such, we only consider *well-formed* programs: those with unique labels across their constituent instructions. For brevity, we drop the instruction labels when they are immaterial to the discussion.

As is standard practice, we use error statements as test oracles to detect violations. In particular, error statements can be used to encode *assert* statements as shown in Fig. 4. Heap-manipulating instructions include allocation, deallocation, lookup and mutation. The $x :=$ `alloc()` instruction allocates a new (unused) location on the heap and returns it in x, and can be used to represent the standard, possibly `null`-returning `malloc()` from C as shown in Fig. 4. Dually, `free(`x`)` deallocates the location denoted by x. Heap lookup $x := [y]$ reads the contents of the location denoted by y and returns it in x; heap mutation $[x] := y$ overwrites the contents of the location denoted by x with y.

Assertions. The *ISL assertion language* is given by the grammar below, where $\oplus \in \{=, \neq, <, \leq, \ldots\}$. We use p, q, r as metavariables for assertions.

$$\begin{aligned} \textsc{Ast} \ni p, q, r ::= {} & \mathsf{false} \mid p \Rightarrow q \mid \exists x.\ p \mid e \oplus e' && \text{classical and Boolean assertions} \\ & \mid \mathsf{emp} \mid e \mapsto e' \mid e \not\mapsto \mid p * q && \text{structural assertions} \end{aligned}$$

As we describe formally in Sect. 4, assertions describe sets of *states*, where each state comprises a (variable) store and a heap. The classical (first-order logic) and Boolean assertions are standard. Other classical connectives can be encoded using existing ones (e.g., $\neg p \triangleq p \Rightarrow \mathsf{false}$). Aside from the highlighted $x \not\mapsto$, structural assertions are as defined in SL [28], and describe a set of states by constraining the shape of the underlying heap. More concretely, emp describes states in which the heap is empty; $e \mapsto e'$ describes states in which the heap comprises a single location denoted by e containing the value denoted by e'; and $p * q$ describes states in which the heap can be split into two disjoint sub-heaps, one satisfying p and the other q. We often write $e \mapsto -$ as a shorthand for $\exists v.\, e \mapsto v$.

As described above, we extend our structural assertions with the *negative* heap assertion $e \not\mapsto$ (read "e is invalidated"). As with its positive counterpart $e \mapsto e'$, the negative assertion $e \not\mapsto$ describes states in which the heap comprises a single location at e. However, whilst $e \mapsto e'$ states that the location at e is allocated (and contains the value e'), $e \not\mapsto$ states that the location at e is *deallocated*.

ISL Proof Rules (Syntactic ISL Triples). We present the ISL proof rules in Fig. 5. As in incorrectness logic [35], the ISL triples are of the form $\vdash [p]\ \mathbb{C}\ [\epsilon : q]$, denoting that *every* state in the *result* assertion q is reachable from *some* state in the *presumption* assertion p with *exit condition* ϵ. That is, for each state σ_q in q, there exists σ_p in p such that executing $\mathbb{C}$ on σ_p terminates with ϵ and yields σ_q. As such, since false describes an empty state set, $[p]\ \mathbb{C}\ [\epsilon : \mathsf{false}]$ is vacuously valid for all p, $\mathbb{C}$, ϵ. Dually, $[\mathsf{false}]\ \mathbb{C}\ [\epsilon : q]$ is always invalid when $q \not\Rightarrow \mathsf{false}$.

An exit condition, $\epsilon \in$ Exit, may be: 1) *ok*, denoting a successful execution; or 2) $er(\mathrm{L})$, denoting an erroneous execution with the error encountered at the L-labeled instruction. Compared to [35], we further annotate our error conditions to track the offending instructions. Moreover, whilst [35] rules only detect explicit errors caused by `error` statements, ISL rules additionally allow us to track errors caused by *memory safety violations*, namely "use-after-free" violations, where a previously deallocated location is subsequently accessed in the program, and "null-pointer-dereference" violations. Although it is straightforward to distinguish between explicit and memory safety errors, for brevity we use $er(\mathrm{L})$ for both.

Thanks to the separation afforded by ISL assertions, compared to incorrectness triples in [35], ISL triples are *local* in that the states described by their presumptions only contain the resources needed by the program. For instance, as `skip` requires no resource for successful execution, the presumption of Skip is simply given by emp, which remains unchanged in the result. Similarly, `assume(`B`)` requires no resource and results in a state satisfying B. The Assign rule is analogous to its SL counterpart. Similarly, $x := *$ in Havoc assigns a nondeterministic value to x. Although these axioms (and Alloc1, Alloc2) ask for a single equality $x = x'$ in their presumption, one can derive more general triples starting from any presumption p by picking a fresh x' and applying the axiom, and the Frame and Cons rules on the equivalent presumption $x = x' * p[x'/x]$.

SKIP
$\vdash [\mathsf{emp}]\ \mathtt{skip}\ [ok : \mathsf{emp}]$

ASSIGN
$\vdash [x{=}x']\ x := e\ [ok : x{=}e[x'/x]]$

HAVOC
$\vdash [x{=}x']\ x := *\ [ok : x{=}v]$

ASSUME
$\vdash [\mathsf{emp}]\ \mathtt{assume}(B)\ [ok : B]$

ERROR
$\vdash [\mathsf{emp}]\ \mathrm{L}{:}\,\mathtt{error}\ [er(\mathrm{L}) : \mathsf{emp}]$

SEQ1
$$\frac{\vdash [p]\ \mathbb{C}_1\ [er(\mathrm{L}) : q]}{\vdash [p]\ \mathbb{C}_1; \mathbb{C}_2\ [er(\mathrm{L}) : q]}$$

SEQ2
$$\frac{\vdash [p]\ \mathbb{C}_1\ [ok : r] \qquad \vdash [r]\ \mathbb{C}_2\ [\epsilon : q]}{\vdash [p]\ \mathbb{C}_1; \mathbb{C}_2\ [\epsilon : q]}$$

LOOP1
$\vdash [p]\ \mathbb{C}^\star\ [ok : p]$

CHOICE
$$\frac{\vdash [p]\ \mathbb{C}_i\ [\epsilon : q] \quad \text{for some } i \in \{1,2\}}{\vdash [p]\ \mathbb{C}_1 + \mathbb{C}_2\ [\epsilon : q]}$$

EXIST
$$\frac{\vdash [p]\ \mathbb{C}\ [\epsilon : q] \quad x \notin \mathsf{fv}(\mathbb{C})}{\vdash [\exists x. p]\ \mathbb{C}\ [\epsilon : \exists x. q]}$$

LOOP2
$$\frac{\vdash [p]\ \mathbb{C}^\star; \mathbb{C}\ [\epsilon : q]}{\vdash [p]\ \mathbb{C}^\star\ [\epsilon : q]}$$

CONS
$$\frac{p' \Rightarrow p \qquad \vdash [p']\ \mathbb{C}\ [\epsilon : q'] \qquad q \Rightarrow q'}{\vdash [p]\ \mathbb{C}\ [\epsilon : q]}$$

DISJ
$$\frac{\vdash [p_1]\ \mathbb{C}\ [\epsilon : q_1] \qquad \vdash [p_2]\ \mathbb{C}\ [\epsilon : q_2]}{\vdash [p_1 \vee p_2]\ \mathbb{C}\ [\epsilon : q_1 \vee q_2]}$$

SUBST
$$\frac{\vdash [p]\ \mathbb{C}\ [\epsilon : q] \qquad y \notin \mathsf{fv}(p, \mathbb{C}, q)}{\vdash [p[y/x]]\ \mathbb{C}[y/x]\ [\epsilon : q[y/x]]}$$

LOCAL
$$\frac{\vdash [p]\ \mathbb{C}\ [\epsilon : q]}{\vdash [\exists x.\ p]\ \mathtt{local}\ x\ \mathtt{in}\ \mathbb{C}\ [\epsilon : \exists x.\ q]}$$

FRAME
$$\frac{\vdash [p]\ \mathbb{C}\ [\epsilon : q] \qquad \mathsf{mod}(\mathbb{C}) \cap \mathsf{fv}(r) = \emptyset}{\vdash [p * r]\ \mathbb{C}\ [\epsilon : q * r]}$$

ALLOC1
$\vdash [x{=}x']\ x := \mathtt{alloc}()\ [ok : x \mapsto -]$

FREE
$\vdash [x \mapsto e]\ \mathrm{L}{:}\,\mathtt{free}(x)\ [ok : x \not\mapsto]$

ALLOC2
$\vdash [x{=}x' * y \not\mapsto]\ x := \mathtt{alloc}()\ [ok : x{=}y * y \mapsto -]$

FREEER
$\vdash [x \not\mapsto]\ \mathrm{L}{:}\,\mathtt{free}(x)\ [er(\mathrm{L}) : x \not\mapsto]$

FREENULL
$\vdash [x{=}\mathtt{null}]\ \mathrm{L}{:}\,\mathtt{free}(x)\ [er(\mathrm{L}) : x{=}\mathtt{null}]$

LOAD
$\vdash [x{=}x' * y \mapsto e]\ \mathrm{L}{:}\,x := [y]\ [ok : x{=}e[x'/x] * y \mapsto e[x'/x]]$

STORE
$\vdash [x \mapsto e]\ \mathrm{L}{:}\,[x] := y\ [ok : x \mapsto y]$

LOADER
$\vdash [y \not\mapsto]\ \mathrm{L}{:}\,x := [y]\ [er(\mathrm{L}) : y \not\mapsto]$

STOREER
$\vdash [x \not\mapsto]\ \mathrm{L}{:}\,[x] := y\ [er(\mathrm{L}) : x \not\mapsto]$

LOADNULL
$\vdash [y{=}\mathtt{null}]\ \mathrm{L}{:}\,x := [y]\ [er(\mathrm{L}) : y{=}\mathtt{null}]$

STORENULL
$\vdash [x{=}\mathtt{null}]\ \mathrm{L}{:}\,[x] := y\ [er(\mathrm{L}) : x{=}\mathtt{null}]$

Fig. 5. The ISL proof rules where x and x' are distinct variables.

Note that `skip`, assignments and assume statements always terminate successfully (with ok). By contrast, $\mathrm{L}{:}\,\mathtt{error}$ always terminates erroneously (with $er(\mathrm{L})$) and requires no resource. The ISL rules SEQ1, SEQ2, CHOICE, LOOP1, LOOP2, CONS, DISJ and SUBST are as in [35]. The SEQ1 rule captures short-circuiting when the first statement ($\mathbb{C}_1$) encounters an error and thus the program terminates erroneously. Analogously, SEQ2 states that when $\mathbb{C}_1$ executes

successfully, the program terminates with ϵ when the subsequent $\mathbb{C}_2$ statement terminates with ϵ. The Choice rule states that the states in q are reachable from p when executing $\mathbb{C}_1 + \mathbb{C}_2$ if they are reachable from p when executing either branch. Loop1 captures immediate exit from the loop; Loop2 states that q is reachable from p when executing $\mathbb{C}^\star$ if it is reachable after a non-zero number of $\mathbb{C}$ iterations.

The Cons rule allows us to strengthen the result and weaken the presumption: if q' is reachable from p', then the smaller q is reachable from the bigger p. Note that compared to SL, the direction of implications in the Cons premise are flipped. Using Cons, we can rewrite the premises of Disj as $[p_1 \vee p_2]\ \mathbb{C}\ [\epsilon : q_1]$ and $[p_1 \vee p_2]\ \mathbb{C}\ [\epsilon : q_2]$. As such, if both q_1 and q_2 are reachable from $p_1 \vee p_2$, then $q_1 \vee q_2$ is also reachable from $p_1 \vee p_2$, as shown in Disj. The Exist rule is derived from Disj; Subst is standard and allows us to substitute x with a fresh variable y; Local is equivalent to that in [35] but uses the Barendregt variable convention, renaming variables in formulas instead of in commands to avoid clashes.

As in SL, the crux of ISL reasoning lies in the Frame rule, allowing one to extend the presumption and the result of a triple with disjoint resources in r. The $\mathsf{fv}(r)$ function returns the set of free variables in r, and $\mathsf{mod}(\mathbb{C})$ returns the set of (program) variables modified by $\mathbb{C}$ (i.e., those on the left-hand of ':=' in assignment, lookup and allocation). These definitions are standard and elided.

Negative assertions allow us to detect memory safety violations when accessing deallocated locations. For instance, FreeEr states that attempting to deallocate x causes an error when x is already deallocated; *mutatis mutandis* for LoadEr and StoreEr. As shown in Alloc2, we can use negative assertions to allocate a previously-deallocated location: if y is deallocated ($y \not\mapsto$ holds in the presumption), then it may be reallocated. The FreeNull, LoadNull and StoreNull rules state that accessing x causes an error when x is `null`. Finally, Load and Store describe the successful execution of heap lookup and mutation, respectively.

Remark 1. Note that mutation and deallocation rules in SL are given as $\{x \mapsto -\}\ [x] := y\ \{x \mapsto y\}$ and $\{x \mapsto -\}\ \texttt{free}(x)\ \{\mathsf{emp}\}$; i.e., the value of x is existentially quantified in the precondition. We can similarly rewrite the ISL rules as:

StoreWeak
$\vdash [x \mapsto -]\ [x] := y\ [ok : x \mapsto y]$

FreeWeak
$\vdash [x \mapsto -]\ \texttt{free}(x)\ [ok : x \not\mapsto]$

However, these rules are too weak. For instance, we cannot use StoreWeak to prove $[x \mapsto 7]\ [x] := y\ [ok : x \mapsto y]$. This is because the implications in the premise of the Cons rule are flipped from those in their SL counterpart, and thus to use StoreWeak we must show $x \mapsto - \Rightarrow x \mapsto 7$ which we cannot. Put differently, StoreWeak states that for *some* value v, executing $[x] := y$ on a state satisfying $x \mapsto v$ yields a state satisfying $x \mapsto y$. However, this statement is valid for *all* values of v. As such, we strengthen the presumption of Store to $x \mapsto e$, allowing for an arbitrary (universally quantified) expression e at x.

In general, in over-approximate logics (e.g., SL) the aim is to *weaken* the preconditions and *strengthen* the postconditions of specifications as much as possible. This is to ensure that we can optimally apply the Cons rule to adapt the specifications to broader contexts. Conversely, in under-approximate logics (e.g., ISL) we should strengthen the presumptions and weaken the results as much as possible, since the implication directions in the premise of Cons are flipped.

Remark 2. The backward reasoning rules of SL [28] are generally unsound for ISL, just as the backward reasoning rules of Hoare logic are unsound for incorrectness logic [35]. For instance, the backward axiom for store is $\{x \mapsto - * (x \mapsto y \mathrel{-\!\!*} p)\}\ [x] := y\ \{p\}$. However, taking $p = \mathsf{emp}$ yields an inconsistent precondition, resulting in the triple $\{\mathsf{false}\}\ [x] := y\ \{\mathsf{emp}\}$, which is valid in SL but not ISL.

Proving. PB-Ok and PB-Client. We next return to the proof sketch of PB-Ok in Fig. 3. For brevity, rather than giving full derivations, we follow the classical Hoare logic proof outline, annotating each line of the code with its presumption and result. We further commentate each proof step and write e.g., //Choice to denote an application of Choice. Note that when applying Choice, we *pick* a branch (e.g., the left branch in PB-Ok) to execute. Observe that unlike in SL where one needs to reason about *all* branches, in ISL it suffices to pick and reason about a *single* branch, and the remaining branches are ignored.

As in Hoare logic proof outlines, we assume that Seq2 is applied at every step; i.e., later instructions are executed only if the earlier ones execute successfully. In most steps, we apply Frame to frame off the unused resource r, carry out the instruction effect, and subsequently frame on r. For instance, when verifying $z := *$ in the proof sketch of PB-Ok, we apply Havoc to pick a non-zero value for z (in this case 1) after the assignment. As such, since the presumption of Havoc is emp, we use Frame to frame off the resource $v \mapsto a{*}a \mapsto -$ in the presumption, apply Havoc to obtain $z = 1$, and subsequently frame on $v \mapsto a{*}a \mapsto -$, yielding $z = 1 * v \mapsto a * a \mapsto -$. For brevity, we keep the applications of Frame and Seq2 implicit and omit them in our annotations. The proof of PB-Client in Fig. 3 is then straightforward and applies the PB-Ok specification when calling `push_back(`v`)`. We refer the reader to the technical appendix [38] where we apply ISL to a further example to detect a null-pointer-dereference bug in OpenSSL.

4 The ISL Model

Denotational Semantics. We present the ISL semantics in Fig. 6. The semantics of a statement $\mathbb{C} \in \text{Comm}$ under an exit condition $\epsilon \in \text{Exit}$, written $[\![\mathbb{C}]\!]\epsilon$, is described as a relation on *program states*. A program state, $\sigma \in \text{State}$, is a pair of the form (s, h), comprising a (variable) *store* $s \in \text{Store}$ and a *heap* $h \in \text{Heap}$.

$$[\![.]\!] : \textsc{Comm} \to \textsc{Exit} \to \mathcal{P}(\textsc{State} \times \textsc{State}) \qquad \sigma \in \textsc{State} \triangleq \textsc{Store} \times \textsc{Heap}$$
$$s \in \textsc{Store} \triangleq \textsc{Var} \xrightarrow{\text{fin}} \textsc{Val} \qquad h \in \textsc{Heap} \triangleq \textsc{Loc} \xrightarrow{\text{fin}} \textsc{Val} \uplus \{\bot\} \qquad l \in \textsc{Loc} \subseteq \textsc{Val}$$

$$[\![\texttt{skip}]\!]ok \triangleq \{(\sigma,\sigma) \mid \sigma \in \textsc{State}\} \qquad [\![\texttt{skip}]\!]er(-) \triangleq \emptyset$$
$$[\![x := e]\!]ok \triangleq \{((s,h),(s[x \mapsto s(e)],h))\} \qquad [\![x := e]\!]er(-) \triangleq \emptyset$$
$$[\![x := *]\!]ok \triangleq \{((s,h),(s[x \mapsto v],h)) \mid v \in \textsc{Val}\} \qquad [\![x := *]\!]er(-) \triangleq \emptyset$$
$$[\![\texttt{assume}(B)]\!]ok \triangleq \{(\sigma,\sigma) \mid \sigma{=}(s,h) \wedge s(B){\neq}0\} \qquad [\![\texttt{assume}(B)]\!]er(-) \triangleq \emptyset$$
$$[\![\textsc{l}\colon \texttt{error}]\!]ok \triangleq \emptyset \qquad [\![\textsc{l}\colon \texttt{error}]\!]er(\textsc{l}') \triangleq \{(\sigma,\sigma) \mid \textsc{l}{=}\textsc{l}'\}$$
$$[\![\mathbb{C}_1;\mathbb{C}_2]\!]\epsilon \triangleq \left\{(\sigma,\sigma') \;\middle|\; \begin{array}{l} \epsilon \neq ok \wedge (\sigma,\sigma') \in [\![\mathbb{C}_1]\!]\epsilon \\ \vee\ \exists \sigma''.\ (\sigma,\sigma'') \in [\![\mathbb{C}_1]\!]ok \wedge (\sigma'',\sigma') \in [\![\mathbb{C}_2]\!]\epsilon \end{array}\right\}$$
$$[\![\texttt{local}\ x\ \texttt{in}\ \mathbb{C}]\!]\epsilon \triangleq \{((s[x \mapsto v],h),(s'[x \mapsto v],h')) \mid ((s,h),(s',h')) \in [\![\mathbb{C}]\!]\epsilon\}$$
$$[\![\mathbb{C}_1 + \mathbb{C}_2]\!]\epsilon \triangleq [\![\mathbb{C}_1]\!]\epsilon \cup [\![\mathbb{C}_2]\!]\epsilon$$
$$[\![\mathbb{C}^\star]\!]\epsilon \triangleq \bigcup_{i\in\mathbb{N}} [\![\mathbb{C}^i]\!]\epsilon \quad \text{with} \quad \mathbb{C}^0 \triangleq \texttt{skip} \quad \text{and} \quad \mathbb{C}^{i+1} \triangleq \mathbb{C};\mathbb{C}^i$$
$$[\![x := \texttt{alloc()}]\!]ok \triangleq \left\{(\sigma,(s[x \mapsto l],h[l \mapsto v])) \;\middle|\; \begin{array}{l} \sigma{=}(s,h) \wedge v \in \textsc{Val} \\ \wedge\ (l \notin dom(h) \vee h(l){=}\bot) \end{array}\right\}$$
$$[\![x := \texttt{alloc()}]\!]er(-) \triangleq \emptyset$$
$$[\![\textsc{l}\colon \texttt{free}(x)]\!]ok \triangleq \{(\sigma,(s,h[s(x) \mapsto \bot])) \mid \sigma{=}(s,h) \wedge h(s(x)) \in \textsc{Val}\}$$
$$[\![\textsc{l}\colon \texttt{free}(x)]\!]er(\textsc{l}') \triangleq \{(\sigma,\sigma) \mid \textsc{l}{=}\textsc{l}' \wedge \sigma{=}(s,h) \wedge (s(x){=}\texttt{null} \vee h(s(x)){=}\bot)\}$$
$$[\![\textsc{l}\colon x := [y]]\!]ok \triangleq \{(\sigma,(s[x \mapsto v],h)) \mid \sigma{=}(s,h) \wedge h(s(y)){=}v \in \textsc{Val}\}$$
$$[\![\textsc{l}\colon x := [y]]\!]er(\textsc{l}') \triangleq \{(\sigma,\sigma) \mid \textsc{l}{=}\textsc{l}' \wedge \sigma{=}(s,h) \wedge (s(y){=}\texttt{null} \vee h(s(y)){=}\bot)\}$$
$$[\![\textsc{l}\colon [x] := y]\!]ok \triangleq \{(\sigma,(s,h[s(x) \mapsto s(y)])) \mid \sigma{=}(s,h) \wedge h(s(x)) \in \textsc{Val}\}$$
$$[\![\textsc{l}\colon [x] := y]\!]er(\textsc{l}') \triangleq \{(\sigma,\sigma) \mid \textsc{l}{=}\textsc{l}' \wedge \sigma{=}(s,h) \wedge (s(x){=}\texttt{null} \vee h(s(x)){=}\bot)\}$$

$$(\!|\mathsf{emp}|\!) \triangleq \{(s,h) \mid dom(h){=}\emptyset\} \qquad (\!|e \mapsto e'|\!) \triangleq \{(s,h) \mid dom(h){=}\{s(e)\} \wedge h(s(e)){=}s(e'){\neq}\bot\}$$

$$(\!|e \not\mapsto |\!) \triangleq \{(s,h) \mid dom(h){=}\{s(e)\} \wedge h(s(e)){=}\bot\} \qquad (\!|p{*}q|\!) \triangleq \{\sigma_p \bullet \sigma_q \mid \sigma_p \in (\!|p|\!) \wedge \sigma_q \in (\!|q|\!)\}$$

$$\text{where} \qquad (s_1,h_1) \bullet (s_2,h_2) \triangleq \begin{cases} (s_1, h_1 \uplus h_2) & \text{if } s_1{=}s_2 \wedge dom(h_1) \cap dom(h_2){=}\emptyset \\ \text{undefined} & \text{otherwise} \end{cases}$$

Fig. 6. The ISL denotational semantics (top); the ISL assertion semantics (bottom).

A store is a function from variables to values. Given a store s, expression e and Boolean expression B, we write $s(e)$ and $s(B)$ for the values to which e and B evaluate under s, respectively. These definitions are standard and omitted.

A heap is a partial function from *locations*, Loc, to $\textsc{Val} \uplus \{\bot\}$. We model heaps as partial functions as they may grow gradually by allocating additional locations. We use the designated value $\bot \notin \textsc{Val}$ to track those locations that have been deallocated. That is, given $l \in \textsc{Loc}$, if $h(l) \in \textsc{Val}$ then l is allocated in h and holds value $h(l)$; and if $h(l) = \bot$ then l has been deallocated. As we demonstrate shortly, we use $\bot$ to model invalidated assertions such as $x \not\mapsto$.

The semantics in Fig. 6 closely corresponds to ISL rules in Fig. 5. For instance, $[\![x := [y]]\!]ok$ underpins Load, while $[\![x := [y]]\!]er(-)$ underpins LoadEr and LoadNull; e.g., if the location at y is deallocated ($h(s(y)) = \bot$), then executing $x := [y]$ terminates erroneously as captured by $[\![x := [y]]\!]er(-)$. The semantics of mutation, allocation and deallocation are defined analogously. As shown, `skip`, assignment and `assume(`B`)` never terminate erroneously (e.g., $[\![\texttt{skip}]\!]er(-) = \emptyset$), and the semantics of their successful execution is standard. The two disjuncts in $[\![\mathbb{C}_1; \mathbb{C}_2]\!]\epsilon$ capture Seq1 and Seq2, respectively. The semantics of $\mathbb{C}_1 + \mathbb{C}_2$ is defined as the union of those of its two branches. The semantics of $\mathbb{C}^\star$ is defined as the union of the semantics of zero or more $\mathbb{C}$ iterations.

Heap Monotonicity. Note that for all $\mathbb{C}$, ϵ and $(\sigma_p, \sigma_q) \in [\![\mathbb{C}]\!]\epsilon$, the (domain of the) underlying heap in σ_p *monotonically grows* from σ_p to σ_q and *never shrinks*. In particular, whilst the heap domain grows via allocation, all other base cases (including deallocation) leave the domain of the heap (i.e., the heap size) unchanged – deallocation merely updates the value of the given location in the heap to $\bot$ and thus does not alter the heap domain. This is in contrast to the original SL model [28], where deallocation *removes* the given location from the heap, and thus the underlying heap may grow or shrink. As we discuss shortly, this monotonicity is the key reason why our model supports a footprint theorem.

ISL Assertion Semantics. The *semantics of ISL assertions* is given at the bottom of Fig. 6 via the function $(\!|.|\!) : \textsc{Ast} \to \mathcal{P}(\textsc{State})$, interpreting each assertion as a set of states. The semantics of classical and Boolean assertions are standard and omitted. As described in Sect. 3, emp describes states in which the heap is empty; and $e \mapsto e'$ describes states of the form (s, h) in which h contains a single location at $s(e)$ with value $s(e')$. Analogously, $e \not\mapsto$ describes states of the form (s, h) in which h contains a single deallocated location at $s(e)$. Finally, the interpretation of $p * q$ contains a state σ iff it can be split into two parts, $\sigma = \sigma_p \bullet \sigma_q$, such that σ_p and σ_q are included in the interpretations of p and q, respectively. The function $\bullet : \textsc{State} \times \textsc{State} \rightharpoonup \textsc{State}$ given at the bottom of Fig. 6 denotes *state composition*, and is defined when the constituent stores agree and the heaps are disjoint. For brevity, we often write $\sigma \in p$ for $\sigma \in (\!|p|\!)$.

Semantic Incorrectness Triples. We next present the formal interpretation of ISL triples. Recall from Sect. 3 that an ISL triple $[p]\ \mathbb{C}\ [\epsilon : q]$ states that every state in q is reachable from some state in p under ϵ. Put formally:

$$\models [p]\ \mathbb{C}\ [\epsilon : q] \overset{\text{def}}{\iff} \forall \sigma_q \in q.\ \exists \sigma_p \in p.\ (\sigma_p, \sigma_q) \in [\![\mathbb{C}]\!]\epsilon$$

Finally, in the following theorem we show that the ISL proof rules are *sound*: if a triple $\vdash [p]\,\mathbb{C}\,[\epsilon : q]$ is derivable using the rules in Fig. 5, then $\models [p]\,\mathbb{C}\,[\epsilon : q]$ holds.

Theorem 1 (Soundness). *For all* $p, \mathbb{C}, \epsilon, q$, *if* $\vdash [p]\ \mathbb{C}\ [\epsilon : q]$, *then* $\models [p]\ \mathbb{C}\ [\epsilon : q]$.

4.1 The Footprint Theorem

The frame rule of SL enables *local* reasoning about a command $\mathbb{C}$ by concentrating only on the parts of the memory that are accessed by $\mathbb{C}$, i.e., the $\mathbb{C}$ *footprint*:

> 'To understand how a program works, it should be possible for reasoning and specification to be confined to the cells that the program actually accesses. The value of any other cell will automatically remain unchanged.' [36]

Local reasoning is then enabled by semantic observations about the local effect of heap accesses. In what follows we describe some of the semantic structure underpinning under-approximate local reasoning, including how it differs from the classic over-approximate theory. Our main result is a footprint theorem, stating that the meaning of a command $\mathbb{C}$ is determined by its action on the "small" part of the memory accessed by $\mathbb{C}$ (i.e., the $\mathbb{C}$ footprint). The overall meaning of $\mathbb{C}$ can then be obtained by "fleshing out" its footprint.

To see this, consider the following example:

1. `free(`y`);`
2. L_2:`free(`y`) + free(`x`);` (FOOT)
3. L_3:`free(`x`) + skip`

For simplicity, let us ignore variable stores for the moment and consider the executions of FOOT from an initial heap $h \triangleq [l_x \mapsto 1, l_y \mapsto 2, l_z \mapsto 3]$, containing locations l_x, l_y and l_z, corresponding to variables x, y and z, respectively. Note that starting from h, FOOT gives rise to four executions depending on the $+$ branches taken at lines 2 and 3. Let us consider the successful execution from h that first frees y, then frees x (the right branch of $+$ on line 2), and finally executes `skip` (the right branch of $+$ on line 3). The footprint of this execution from h is then given by $(ok : [l_x \mapsto 1, l_y \mapsto 2], [l_x \mapsto \bot, l_y \mapsto \bot])$, denoting an *ok* execution from the initial sub-heap $[l_x \mapsto 1, l_y \mapsto 2]$, yielding the final sub-heap $[l_x \mapsto \bot, l_y \mapsto \bot]$ upon termination. That is, the initial and final sub-heaps in the footprint do not include the untouched location l_z as it remains unchanged, and the overall effect of FOOT is obtained from its footprint by adding $l_z \mapsto 3$ to both the initial and final sub-heaps; i.e., by "fleshing out" the footprint.

Next, consider the execution in which the left branch of $+$ on line 2 is taken, resulting in a use-after free error. The footprint of this second execution from h is given by $(er(\text{L}_2) : [l_y \mapsto 2], [l_y \mapsto \bot])$, denoting an error at L_2. Note that as this execution terminates erroneously at L_2, unlike in the first execution, location l_x remains untouched by FOOT and is thus not included in the footprint.

Put formally, let `foot`$(.) : \text{Comm} \to \text{Exit} \to \mathcal{P}(\text{State} \times \text{State})$ denote a *footprint function* such that `foot`$(\mathbb{C})\,\epsilon$ describes the *minimal* state needed for *some* $\mathbb{C}$ execution under ϵ: if $((s,h),(s',h')) \in$ `foot`$(\mathbb{C})\,\epsilon$, then h contains only the locations accessed by some $\mathbb{C}$ execution, yielding h' on termination. In Fig. 7 we present an excerpt of `foot`$(.)$, with its full definition given in [38].

$$\begin{aligned}
\texttt{foot}\,(\mathbb{C}_1 + \mathbb{C}_2)\,\epsilon &\triangleq \texttt{foot}\,(\mathbb{C}_1)\,\epsilon \cup \texttt{foot}\,(\mathbb{C}_2)\,\epsilon \\
\texttt{foot}\,(\text{L}\colon \texttt{free}(x))\,ok &\triangleq \left\{ \left((s, [l \mapsto v]), (s, [l \mapsto \bot])\right) \mid s(x){=}l \wedge v \in \text{VAL} \right\} \\
\texttt{foot}\,(\text{L}\colon \texttt{free}(x))\,er(\text{L}') &\triangleq \left\{ \left((s, [l \mapsto \bot]), (s, [l \mapsto \bot])\right) \mid \text{L}{=}\text{L}' \wedge s(x){=}l \right\} \\
&\quad \cup \left\{ \left((s, h_0), (s, h_0)\right) \mid \text{L}{=}\text{L}' \wedge s(x){=}\texttt{null} \right\}
\end{aligned}$$

Fig. 7. The `foot` (.) function (excerpt), where h_0 denotes an empty heap ($dom(h_0) = \emptyset$).

Our footprint theorem (Theorem 2) then states that any pair (σ_p, σ_q) resulting from executing $\mathbb{C}$ (i.e., $(\sigma_p, \sigma_q) \in [\![\mathbb{C}]\!]\epsilon$) can be obtained by fleshing out a pair (σ'_p, σ'_q) in the $\mathbb{C}$ footprint (i.e., $(\sigma'_p, \sigma'_q) \in \texttt{foot}\,(\mathbb{C})\,\epsilon$): $(\sigma_p, \sigma_q) = (\sigma'_p \bullet \sigma_r, \sigma'_q \bullet \sigma_r)$ for some σ_r.

Theorem 2 (Footprints). *For all* $\mathbb{C}$ *and* ϵ: $[\![\mathbb{C}]\!]\epsilon = \texttt{frame}\,(\texttt{foot}\,(\mathbb{C})\,\epsilon)$, *where* $\texttt{frame}\,(R) \triangleq \left\{ (\sigma_p \bullet \sigma_r, \sigma_q \bullet \sigma_r) \mid (\sigma_p, \sigma_q) \in R \right\}$.

We note that our footprint theorem is a positive by-product of the ISL *model* and *not* the ISL logic. That is, the footprint theorem is an added bonus of the heap monotonicity in the ISL model, brought about by negative heap resources, and is orthogonal to the notion of under-approximation. As such, the footprint theorem would be analogously valid in the original SL model, were we to alter its model to achieve heap monotonicity through negative heaps. That said, there are important differences with the classic SL theory, which we discuss next.

4.2 Differences with the Classic (Over-Approximate) Theory

Existing work [14,40] presents footprint theorems for classical SL based on the notion of *safe states*; i.e., those that do not lead to erroneous executions. This is understandable as the informal reasoning which led to the frame rule for SL was based on safety [36,45]. According to the *fault-avoiding interpretation* of an SL triple $\{p\}\,\mathbb{C}\,\{q\}$, deemed invalid when a state in p leads to an error, if $\mathbb{C}$ accesses a location outside p, then this leads to a safety violation. As such, any location not guaranteed to exist in p must remain unchanged, thereby yielding the frame rule. The existing footprint theorems were for safe states only.

By contrast, our theorem considers footprints involving both unsafe and safe states. For instance, given the FOOT program and an initial state (e.g., h in Sect. 4.1), we distinguished a footprint leading to an erroneous execution (e.g., $(er(\text{L}_2) : [l_y \mapsto 2], [l_y \mapsto \bot])$) from one leading to a safe execution (e.g., $(ok : [l_x \mapsto 1, l_y \mapsto 2], [l_x \mapsto \bot, l_y \mapsto \bot])$). This distinction is important, as otherwise we could not distinguish further bugs that follow a safe execution. To see this, consider a second error in FOOT, namely the possible use-after-free of x on line 3, following a successful execution of lines 1 and 2.

For reasoning about incorrectness, it is essential that we consider unsafe states when accounting for why things work; this is a technical difference with the classic footprint results. But it also points to a deeper conceptual difference

between the correctness and incorrectness theories. Above, we explained how safety, and its violation, played a crucial role in justifying the frame rule of over-approximate SL. However, as we describe below, ISL and its frame rule do not rely on safety.

As shown in [35], an under-approximate triple can be equivalently defined as: $[p]\,\mathbb{C}\,[\epsilon : q] \overset{\text{def}}{\iff} \mathsf{post}(\mathbb{C}, p) \supseteq q$, where $\mathsf{post}(\mathbb{C}, p)$ describes the states obtained by executing $\mathbb{C}$ on p. While this under-approximate definition equivalently justifies the frame rule, the analogous over-approximate (Hoare) triple obtained by flipping $\supseteq$ (i.e., $\{p\}\,\mathbb{C}\,\{q\} \overset{\text{def}}{\iff} \mathsf{post}(\mathbb{C}, p) \subseteq q$) invalidates the frame rule:

$$\frac{\{\mathsf{true}\}[x] := 23\{\mathsf{true}\}}{\{x \mapsto 17 * \mathsf{true}\}[x] := 23\{x \mapsto 17 * \mathsf{true}\}}\ (\textsc{Frame})$$

The premise of this derivation is valid according to the standard interpretation of over-approximate triples, but its conclusion (obtained by framing on $x \mapsto 17$) certainly is not, as it states that the value of x remains unchanged after mutation.

The frame rule is then recovered by strengthening the $\{p\}\,\mathbb{C}\,\{q\}$ interpretation, *either* by requiring that executing $\mathbb{C}$ on p not fault (fault avoidance), *or* by "baking in" frame preservation: $\forall r.\ \mathsf{post}(\mathbb{C}, p * r) \subseteq q * r$. Both solutions then invalidate the premise of the above derivation. We found it remarkable that our ISL theory is consistent with the technically simpler interpretation of triples – namely as $\mathsf{post}(\mathbb{C}, p) \supseteq q$, the dual of Hoare's interpretation – and that it supports a simple footprint theorem at once, again in contrast to the over-approximate theory.

5 Begin-Anywhere, Intra-procedural Symbolic Execution

ISL lends itself naturally to the definition of forward symbolic execution analyses. We demonstrate that using the ISL rules, it is straightforward to derive a *begin-anywhere*, *intra-procedural* analysis that allows us to infer valid ISL triples *automatically* for a given piece of code, with the goal of finding only true bugs reachable from an initial state. This is implemented in the intra-procedural-only mode of the Pulse analysis inside Infer [18] (accessible by passing `--pulse --pulse-intraprocedural-only` to `infer`). The analysis follows principles from bi-abduction [11], but takes its most successful application – bug catching [18] – as the sole objective. This allows us to make a number of adjustments and to obtain an analysis that is a much closer fit to the ISL theory of under-approximation than the original bi-abduction analysis was to the SL theory of over-approximation.

The original bi-abduction analysis in Abductor [11] and Infer [18] aimed at discovering fault-avoiding specifications for procedures. Ideally, one would find specifications for *all* procedures in the codebase, all the way to an entry-point (e.g., the `main()` function), thus proving the program safe. In practice, however, virtually all sizable codebases have bugs, and known abstract domains are imprecise when proving memory safety for large codebases. As such, specifications were

$p, q ::= \mathsf{emp} \mid e \oplus e' \mid e \mapsto e' \mid e \not\mapsto \mid p * q$ Symbolic Heaps

$$\textsc{SE-Seq}\quad \frac{[p_0]\,\mathbb{C}_0\,[ok : q_0]\;\mathbb{C}_1 \rightsquigarrow [p_1]\;\mathbb{C}_0; \mathbb{C}_1\;[\epsilon_1 : q_1] \quad [p_1]\,\mathbb{C}_0; \mathbb{C}_1\,[\epsilon_1 : q_1]\;\mathbb{C}_2 \rightsquigarrow [p_2]\;\mathbb{C}_0; \mathbb{C}_1; \mathbb{C}_2\;[\epsilon_2 : q_2]}{[p_0]\,\mathbb{C}_0\,[ok : q_0]\;\mathbb{C}_1; \mathbb{C}_2 \rightsquigarrow [p_2]\;\mathbb{C}_0; \mathbb{C}_1; \mathbb{C}_2\;[\epsilon_2 : q_2]}$$

$$\textsc{SE-Choice}\quad \frac{[p_0]\,\mathbb{C}_0\,[ok : q_0]\;\mathbb{C}_i \rightsquigarrow [p_i]\;\mathbb{C}_0; \mathbb{C}_i\;[\epsilon_i : q_i]}{[p_0]\,\mathbb{C}_0\,[ok : q_0]\;\mathbb{C}_1 + \mathbb{C}_2 \rightsquigarrow [p_i]\;\mathbb{C}_0; \mathbb{C}_1 + \mathbb{C}_2\;[\epsilon_i : q_i]}$$

$$\textsc{SE-Store}\quad \frac{q * M \dashv x \mapsto e * F \qquad \mathsf{mod}(\mathbb{C}) \cap \mathsf{fv}(M) = \emptyset}{[p]\,\mathbb{C}\,[ok : q]\;\;[x] := y \rightsquigarrow [p * M]\,\mathbb{C}; [x] := y\,[ok : x \mapsto y * F]}$$

$$\textsc{SE-StoreEr}\quad \frac{q \vdash x \not\mapsto \;* \mathsf{true} \text{ or } q \vdash x = \mathtt{null} * \mathsf{true}}{[p]\,\mathbb{C}\,[ok : q]\;\textsc{l}\colon [x] := y \rightsquigarrow [p]\;\mathbb{C}; \textsc{l}\colon [x] := y\;[er(\textsc{l}) : q]}$$

Fig. 8. Symbolic heaps (above) and selected symbolic execution rules (below).

found for only 40–70% of the procedures in the experiments of [11]. Nonetheless, proof failures, a by-product of proof search, became practically more valuable than proofs, as they can indicate errors. Complex heuristics came into play to classify proof failures and to report to the programmer those more likely to be errors. These heuristics have not been given a formal footing, contributing to the gap between the theory of proofs and the practice of bug catching.

Pulse approaches bug reporting more directly: by looking for them. It infers under-approximate specifications, while recording invalidated addresses. If such an address is later accessed, a bug is reported soundly, in line with the theory.

Symbolic Execution. In Fig. 8 we present our symbolic execution as big-step, syntax-directed inference rules of the form $[p_0]\,\mathbb{C}_0\,[\epsilon_0 : q_0]\;\mathbb{C} \rightsquigarrow [p]\;\mathbb{C}_0; \mathbb{C}\;[\epsilon : q]$, which can be read as: "having already executed $\mathbb{C}_0$ yielding (discovering) the presumption p_0 and the result q_0, then executing $\mathbb{C}$ yields the presumption p and result q". As is standard in SL-based tools [4,11], our abstract states consist of $*$-conjoined predicates, with the notable addition of the invalidated assertion and omission of inductive predicates. The latter are not needed because we never perform the over-approximation steps that would introduce them.

SE-Seq describes how the symbolic execution goes forward step by step. SE-Choice describes how the analysis computes one specification per path taken in the program. To ensure termination, loops are unrolled up to a fixed bound N_{loops}, borrowing from symbolic bounded model checking [12]. These two ideas avoid the arduous task of inventing join and widen operators [15]. For added efficiency, in practice we also limit the maximum number of paths leading to the same program point to a fixed bound $N_{\text{disjuncts}}$. The N_{loops} and $N_{\text{disjuncts}}$bounds

give us easy "knobs" to tune the precision of the analysis. Note that pruning paths by limiting disjuncts is also sound for under-approximate reasoning [35].

To analyze a program $\mathbb{C}$, we start from $\mathbb{C}_0 = \texttt{skip}$ and produce $[\mathsf{emp}]\ \texttt{skip}\ [ok : \mathsf{emp}]\ \mathbb{C} \rightsquigarrow [p]\ \texttt{skip}; \mathbb{C}\ [\epsilon : q]$. As $\models [\mathsf{emp}]\ \texttt{skip}\ [ok : \mathsf{emp}]$ holds and symbolic execution rules preserve validity, we then obtain valid triples for $\mathbb{C}$ by Theorem 3.

Theorem 3 (Soundness of Symbolic Execution). *If* $\models [p_0]\ \mathbb{C}_0\ [\epsilon : q_0]$ *and* $[p_0]\ \mathbb{C}_0\ [\epsilon : q_0]\ \mathbb{C} \rightsquigarrow [p]\ \mathbb{C}_0; \mathbb{C}\ [\epsilon : q]$, *then* $\models [p]\ \mathbb{C}_0; \mathbb{C}\ [\epsilon : q]$.

Symbolic execution of individual commands follows the derived SymbExec rule below, with the side-condition that $\mathsf{mod}(\mathbb{C}_0) \cap \mathsf{fv}(M) = \mathsf{mod}(\mathbb{C}) \cap \mathsf{fv}(F) = \emptyset$:

$$\textsc{SymbExec}\quad \frac{\dfrac{[p_0]\ \mathbb{C}_0\ [ok : q_0]}{[p_0 * M]\ \mathbb{C}_0\ [ok : q_0 * M]} \qquad q_0 * M \dashv p * F \qquad \dfrac{[p]\ \mathbb{C}\ [\epsilon : q]}{[p * F]\ \mathbb{C}\ [\epsilon : q * F]}}{[p_0 * M]\ \mathbb{C}_0; \mathbb{C}\ [\epsilon : q * F]}$$

If executing $\mathbb{C}_0$ yields the presumption p_0 and the current state q_0, then SymbExec allows us to execute the next command $\mathbb{C}$ with specification $[p]\ \mathbb{C}\ [\epsilon : q]$. This may 1) materialize a state M that is *missing* from q_0 (and is needed to execute $\mathbb{C}$); and 2) carry over an unchanged *frame* F. The unknowns M and F in the *bi-abduction question* $p * F \vdash q_0 * M$ have analogous counterparts in over-approximate bi-abduction; but, as in the Cons rule, their roles have flipped: the *frame* F is *abduced*, while the missing M is *framed* (or *anti-abduced*).

Bi-abduction and ISL. Bi-abduction is arguably a better fit for ISL than SL: in SL adding the missing M to the overall precondition p_0 is only valid for straight-line code, and not across control flow branches. Intuitively, there is no guarantee that a safe precondition for one path is safe for the other. This is especially the case in the presence of non-determinism or over-approximation of Boolean conditions, where one cannot find definitive predicates to force the analysis down one path. It is thus necessary to *re-execute* the whole procedure on the inferred preconditions, eliminating those that are not safe for all paths. By contrast, in our setting SE-Choice is *sound*, and this re-execution is not needed!

We allow the analysis to abduce information only for *successful* execution; *erroneous* executions have to be *manifest* and realizable using only the information at hand. We do this by requiring M to be emp in SymbExec when applied to error triples. We go even further and require that the implication be in both directions, i.e., that the current state *force* the error – note that if $q \vdash x \not\mapsto * \mathsf{true}$ then there exists F such that $x \not\mapsto * F \vdash q$, and similarly for $q \vdash x = \texttt{null} * \mathsf{true}$. This is a practical choice and only one of many ways to decide *where* to report, trying to avoid blaming the code for issues it did not itself cause. For instance, thanks to this restriction, we do not report on $[x] := 10$ (which has error specifications through StoreEr and StoreNull) unless a previous instruction actively invalidated x. This choice also chimes well with the fact that the analysis can *start anywhere* in a program and give results relevant to the code analyzed.

Solving the bi-abduction entailment in SymbExec can be done using the techniques developed for SL [11, §3]. We do not detail them here as they are straightforwardly adapted to our simpler setting without inductive predicates.

Finding a Bug in `client`, Automatically. We now describe how Pulse automatically finds a proof of the bug in the unnanotated code of `client` from Fig. 3, by automatically applying the only possible symbolic execution rule at each step. Starting from emp and going past the first instruction $x := [v]$ requires solving $v \mapsto u * F \vdash \mathsf{emp} * M$. The bi-abduction entailment solver then answers with $F = \mathsf{emp}$ and $M = v \mapsto u$, yielding the inferred presumption $v \mapsto u$ and the next current state $v \mapsto u * x = u$. The next instruction is the call to `push_back(`v`)`. For ease of presentation, let us consider this library call as an axiomatized instruction that has been given the specification in Fig. 3. This corresponds to writing a model for it in the analyzer, which is actually the case in the implementation, although the analysis would work equally well if we were to inline the code inside `client`. Applying SymbExec requires solving the entailment $v \mapsto a * a \mapsto w * F \vdash v \mapsto u * x = u * M$. The solver then answers with the solution $F = (x = u * a = u)$ and $M = u \mapsto w$. Finally, the following instance of SE-StoreEr is used to report an error, where $\mathbb{C} = \texttt{skip}; x := [v]; \texttt{push\_back}(v)$ and $q_{rx} = v \mapsto a' * a' \mapsto w * a \not\mapsto * x = u * a = u$:

$$[v \mapsto u * u \mapsto w]\ \mathbb{C}\ [ok : q_{rx}]\ \mathrm{L}_{rx} : [x] := 88$$
$$\rightsquigarrow [v \mapsto u * u \mapsto w]\ \mathbb{C}; \mathrm{L}_{rx} : [x] := 88\ [er(\mathrm{L}_{rx}) : q_{rx}]$$

Preliminary Results. Our analysis handles the examples in this paper, modulo function inlining. While our analysis shows how to derive a sound static analysis from first principles, it does not yet fully exploit the theory, as it does not handle function calls, and in particular *summarization*. Under-approximate triples pave the way towards succinct summaries. However, this is a subtle problem, requiring significant theoretical and empirical work out of the scope of this initial paper.

Pragmatically, we can make Pulse scale by skipping over procedure calls instead of inlining them, in effect assuming that the call has no effect beyond assigning fresh (non-deterministic) values to the return address and the parameters passed by reference – note that such fresh values are treated optimistically by Pulse as we do not know them to be invalid. In theory, this may cause false positives and false negatives, but in practice we observed that such an analysis reports very few issues. For instance, it reports no issues on OpenSSL 1.0.2d (with 8681 C functions) at the time of writing, and only 17 issues on our proprietary C++ codebase of hundreds of thousands of procedures. As expected, the analysis is very fast and scales well (6 s for OpenSSL, running on a Linux machine with 24 cores). Moreover, 30 disjuncts suffice to detect all 17 issues (in comparison, using 20 disjuncts misses 1 issue, while using 100 disjuncts detects no more issues than using 30 disjuncts), and varying loop unrollings between 1–10 has no effect.

We also ran Pulse in production at Facebook and reported issues to developers as they submit code changes, where bugs are more likely than in mature

codebases. Over the course of 4 months, Pulse reported 20 issues to developers, of which 15 were fixed. This deployment relies crucially on the begin-anywhere capability: though the codebase in question has 10s of MLOC, analysing a code change starts from the changed files and usually visits only a small fraction of the codebase.

Under-Approximation in Pulse. Pulse achieves under-approximate reasoning in several ways. First, Pulse uses the under-approximate Choice, Loop1 and Loop2 rules in Fig. 5 which prune paths by considering one execution branch (Choice) or finite loop unrollings (Loop1 and Loop2). Second, Pulse does not use Alloc2, and thus prunes further paths. Third, Pulse uses under-approximate models of certain library procedures; e.g., the `vector::push_back()` model assumes the internal array is always deallocated. Finally, our bi-abduction implementation assumes that memory locations are distinct unless known otherwise, thus leading to further path pruning. These choices are all sound thanks to the under-approximate theory of ISL; it is nevertheless possible to make different pragmatic choices.

Although our implementation does not do it, we can use ISL to derive strongest posts for primitive statements, using a combination of their axioms and the Frame, Disj and Exist rules. Given the logic fragment we use (which excludes inductive predicates) and a programming language with Boolean conditions restricted to a decidable fragment, there is likely a bounded decidability result obtained by unrolling loops up to a given bound and then checking the strongest post on each path. However, the ability to under-approximate (by forgetting paths/disjuncts) gives us the leeway to tune a deployment for optimizing the bugs/minute rate: in one experiment, we found that running Pulse on a codebase with 100s kLOC and a limit of 20 disjuncts was ∼3.1x user-time faster than running it with a limit of 50 disjuncts, and yet found 97% of the issues found in the 50-disjuncts case.

Remark 3. Note that although the underlying heaps in ISL grow monotonically, the impact on the size of the manipulated states in our analysis is comparable to that of the original bi-abductive analysis for SL [11]. This is in part thanks to the compositionality afforded by ISL and its footprint property (Theorem 2), especially when individual procedures analyzed are not too big. In particular, the original bi-abduction work for SL already tracks the allocated memory; in ISL we additionally track deallocated memory which is of the same order of magnitude.

6 Context, Related Work and Conclusions

Although the foundations of program verification have been mostly developed with correctness in mind, industrial uses of symbolic reasoning often derive value from their deployment as *bug catchers* rather than *provers* of bug absence. There is a fundamental tension in correctness-based techniques, most thoroughly explored in the model checking field, between compact representations versus

strength and utility of counter-examples. Abstraction techniques are typically used to increase compactness. This has the undesired side-effect that counter-examples become "abstract": they may be infeasible, in that they may not actually witness a concrete execution that violates a given property. Using proofs of bugs, this paper aims to provide a symbolic mechanism to express the *definite* existence of a concrete counter-example, without committing to a particular one, while simultaneously enabling sound, compositional, local reasoning. Our working hypothesis is that bugs are a fundamental enough phenomenon to warrant a fundamental compositional theory for reasoning positively about their existence, rather than only being about failed proofs. We hope that future work will explore the practical ramifications of these foundational ideas more thoroughly.

Amongst static bug-catching techniques, there is a dichotomy between the highly scalable, compositional static tools such as Coverity [5], Facebook Infer [18] and those deployed at Google [42], which suffer from false positives as well as negatives, and the under-approximating global bug hunters such as fuzzers [23] and symbolic executors [9], which suffer from scalability limitations but not false positives (at least, ideally). In a recent survey, Godefroid remarks "How to engineer exhaustive symbolic testing (that is, a form of verification) in a cost-effective manner is still an open problem for large applications" [23]. The ability to apply compositional analyses incrementally to large codebases has led to considerable impact that is complementary to that of the global analyses. But, compositional techniques can have less precision compared to global ones: examining all call sites of a procedure can naturally lead to more precise results.

Our illustrative analysis, Pulse, starts from the scalable end of the spectrum and moves towards the under-approximate end. An equally valid research direction would be to start from existing under-approximate analyses and make them more scalable and with lower start-up-cost. There has indeed been valuable research in this direction. For example, SMART [22] tries to make symbolic execution more scalable by using summaries as in inter-procedural static analysis, and UC-KLEE [39] allows symbolic execution to begin anywhere, and thus does not need a complete program. UC-KLEE uses a "lazy initialization" mechanism to synthesize assumptions about data structures; this is not unlike the bi-abductive approach here and in [10]. An interesting research question is whether this similarity can be made rigorous. There are many papers on marrying under- and over-approximation e.g., [1], but they often lack the scalability that is crucial to the impact of modular bug catchers. In general, there is a large unexplored territory, relevant to Godefroid's open problem stated above, between the existing modular but not-quite-under-approximate bug catchers such as Infer and Coverity, and the existing global and under-approximate tools such as KLEE [8], CBMC [12] and DART [24]. This paper provides not a solution, but a step in the exploration.

Gillian [20] is a platform for developing symbolic analysis tools using a symbolic execution engine based on separation logic. Gillian has C and JavaScript instantiations for precise reasoning about a finite unwinding of a program, similar to symbolic bounded model checking. Gillian's execution engine is currently

exact for primitive commands (it is both over- and under-approximate); however, it uses over-approximate bi-abduction for function calls, and is thus open to false positives (Petar Maksimović, personal communication). We believe Gillian can be modified to embrace under-approximation more strongly, serving as a general engine for proving ISL specifications. Aiming for under-approximate results rather than exact ones gives additional flexibility to the analysis designer, just as aiming for over-approximate rather than exact results does for correctness tools.

Many assertion languages for heap reasoning have been developed, including ones not based on SL (e.g., [3,27,31,46]). We do not claim that, compared to these alternatives, the ISL assertion language in this paper is particularly advantageous for reasoning along individual paths, or exhaustive (but bounded) reasoning about complete programs. Rather, the key point is that our analysis solves abduction and anti-abduction problems, which in turn facilitates its application to large codebases. In particular, as our analysis synthesizes contextual heap assumptions (using anti-abduction), it can begin anywhere in a codebase instead of starting from `main()`. For example, it can start on a modified function that is part of a larger program: this capability enables continuous deployment in codebases with millions of LOC [18,34]. To our knowledge, the cited assertion languages have only ever been applied in a whole-program fashion on small codebases (with low thousands of LOC). We speculate that this is not because of the assertion languages *per se*: if methods to solve analogues of abduction and anti-abduction queries were developed, perhaps they too could be applied to large codebases.

It is natural to consider how the ideas of ISL extend to concurrency. The RacerD analyzer [25] provided a static analysis for data races in concurrent programs; this analysis was provably under-approximate under certain assumptions. RacerD was intuitively inspired by concurrent separation logic (CSL [6]), but did not match the over-approximate CSL theory (just as Infer did not match SL). We speculate that RacerD and other concurrency analyses might be seen as constructing proofs in a yet-to-be-defined incorrectness version of CSL, a logic which would aim at finding bugs in concurrent programs via modular reasoning.

Our approach supports reasoning that is local not only in code, but also in state (spatial locality). Spatially local symbolic heap update has led to advances in scalability of global shape analyses of mutable data structures, where heap predicates are modified in-place in a way reminiscent of operational in-place update, and where transfer functions need not track global heap information [44]. Mutable data structures have been suggested as one area where classic symbolic execution has scaling challenges, and SL has been employed with human-directed proof on heap-intensive components to aid the overall scalability of symbolic execution [37]. An interesting question is whether spatial locality in the analysis can benefit scalability of fully automatic, global, under-approximate analyses.

We probed the semantic fundamentals underpinning local reasoning in Sect. 4, including a footprint theorem (Theorem 2) that is independent of the logic. The semantic principles are more deeply fundamental than the surface

syntax of the logic. Indeed, in the early days of work on SL, it was remarked that local reasoning flows from locality properties of the semantics, and that separation logic is but one convenient syntax to exploit these [45]. Since then, a number of correctness logics with non-SL syntax have been proposed for local reasoning (e.g., [33] and its references) that exploit the semantic locality of heap update, and it stands to reason that the same will be possible for incorrectness logics.

Relating this paper to the timeline of SL for correctness, we have developed the basic logic (like [36] but under-approximate) and a simple local intra-procedural analysis (like [19] but under-approximate). We have not yet made the next steps to relatively-scalable global analyses [44] or extremely-scalable inter-procedural, compositional ones [11]. These future directions are challenging for theory and especially practice, and are the subject of ongoing and future work.

Conclusions. Long ago, Dijkstra (in)famously remarked that "testing can be quite effective for showing the presence of bugs, but is hopelessly inadequate for showing their absence" [17], and he advocated the use of logic for the latter. As noted by others, many of the benefits of logic hold for both bug catching and verification, particularly the ability to cover many states and paths succinctly, even if not the alluring all. But there remains a frustrating division between testing and verification, where e.g., distinct tools are used for each. With more research on the fundamentals of symbolic bug catching and correctness, division may be replaced by unified foundations and toolsets in the future. For under-approximate reasoning in particular, we hope that bug catching eventually becomes more modular, scalable, easier to deploy and with elegant foundations similar to those of verification. This paper presents but one modest step towards that goal.

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Stochastic Systems

Maximum Causal Entropy Specification Inference from Demonstrations

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Abstract. In many settings, such as robotics, demonstrations provide a natural way to specify tasks. However, most methods for learning from demonstrations either do not provide guarantees that the learned artifacts can be safely composed or do not explicitly capture temporal properties. Motivated by this deficit, recent works have proposed learning Boolean *task specifications*, a class of Boolean non-Markovian rewards which admit well-defined composition and explicitly handle historical dependencies. This work continues this line of research by adapting maximum *causal* entropy inverse reinforcement learning to estimate the posteriori probability of a specification given a multi-set of demonstrations. The key algorithmic insight is to leverage the extensive literature and tooling on reduced ordered binary decision diagrams to efficiently encode a time unrolled Markov Decision Process. This enables transforming a naïve algorithm with running time exponential in the episode length, into a polynomial time algorithm.

1 Introduction

In many settings, episodic demonstrations provide a natural and robust mechanism to partially specify a task, even in the presence of errors. For example, consider the agent operating in the gridworld illustrated in Fig. 1. Blue arrows denote intended actions and the solid black arrow shows the agent's actual path. This path can stochastically differ from the blue arrows due to a downward wind. One might naturally ask: "What task was this agent attempting to perform?" Even without knowing if this was a positive or negative example, based on the agent's state/action sequence, one can reasonably infer the agent's intent, namely, "reach the yellow tile while avoiding the red tiles." Compared with traditional learning from positive and negative examples, this is somewhat surprising, particularly given that the task is never actually demonstrated in Fig. 1.

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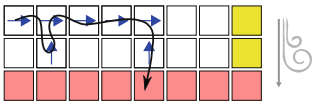


Fig. 1. Example of an agent unsuccessfully demonstrating the task "reach a yellow tile while avoiding red tiles". (Color figure online)

This problem, inferring intent from demonstrations, has received a fair amount of attention over the past two decades particularly within the robotics community [5,22,30,33]. In this literature, one traditionally models the demonstrator as operating within a dynamical system whose transition relation only depends on the current state and action (called the Markov condition). However, even if the dynamics are Markovian, many tasks are naturally modeled in history dependent (non-Markovian) terms, e.g., "if the robot enters a blue tile, then it must touch a brown tile *before* touching a yellow tile". Unfortunately, most methods for learning from demonstrations either do not provide guarantees that the learned artifacts (e.g. rewards) can be safely composed or do not explicitly capture history dependencies [30].

Motivated by this deficit, recent works have proposed specializing to **task specifications**, a class of Boolean non-Markovian rewards induced by formal languages. This additional structure admits well-defined compositions and explicitly captures temporal dependencies [15,30]. A particularly promising direction has been to adapt maximum entropy inverse reinforcement learning [33] to task specifications, enabling a form of robust specification inference, even in the presence unlabeled demonstration errors [30].

However, while powerful, the principle of maximum entropy is limited to settings where the dynamics are deterministic or agents that use open-loop policies [33]. This is because the principle of maximum entropy incorrectly allows the agent's predicted policy to depend on future state values resulting in an overly optimistic agent [19]. For instance, in our gridworld example (Fig. 1), the principle of maximum entropy would discount the possibility of slipping, and thus we would not forecast the agent to correct its trajectory after slipping once.

This work continues this line of research by instead using the principle of maximum *causal* entropy, which generalizes the principle of maximum entropy to general stochastic decision processes [32]. While a conceptually straightforward extension, a naïve application of maximum *causal* entropy inverse reinforcement learning to non-Markovian rewards results in an algorithm with run-time exponential in the episode length, a phenomenon sometimes known as the **curse of history** [24]. The key algorithmic insight in this paper is to leverage the extensive literature and tooling on Reduced Ordered Binary Decision Diagrams (BDDs) [3] to efficiently encode the time unrolled composition of the dynamics and task specification. This allows us to translate a naïve exponential time algorithm into a polynomial time algorithm. In particular, we shall show that this BDD has size at most linear in the episode length making inference comparatively efficient.

1.1 Related Work

Our work is intimately related to the fields of Inverse Reinforcement Learning and Grammatical Inference. **Grammatical inference** [8] refers to the well-developed literature on learning a formal grammar (often an automaton) from data. Examples include learning the smallest automata that in consistent with a set of positive and negative strings [7,8] or learning an automaton using membership and equivalence queries [1]. This and related work can be seen as extending these methods to unlabeled and potentially noisy demonstrations, where demonstrations differ from examples due to the existence of a dynamics model. This notion of demonstration derives from the Inverse Reinforcement Learning literature.

In **Inverse Reinforcement Learning** (IRL) [22] the demonstrator, operating in a stochastic environment, is assumed to attempt to (approximately) optimize some unknown reward function over the trajectories. In particular, one traditionally assumes a trajectory's reward is the sum of state rewards of the trajectory. This formalism offers a succinct mechanism to encode and generalize the goals of the demonstrator to new and unseen environments.

In the IRL framework, the problem of learning from demonstrations can then be cast as a Bayesian inference problem [25] to predict the most probable reward function. To make this inference procedure well-defined and robust to demonstration/modeling noise, Maximum Entropy [33] and Maximum Causal Entropy [32] IRL appeal to the principles of maximum entropy [13] and maximum causal entropy respectively [32]. This results in a likelihood over the demonstrations which is no more committed to any particular behavior than what is required to match observed statistical features, e.g., average distance to an obstacle. While this approach was initially limited to rewards represented as linear combinations of scalar features, IRL has been successfully adapted to arbitrary function approximators such as Gaussian processes [20] and neural networks [5]. As stated in the introduction, while powerful, traditional IRL provides no principled mechanism for composing the resulting rewards.

Compositional RL: To address this deficit, composition using soft optimality has recently received a fair amount of attention; however, the compositions are limited to either strict disjunction (do X *or* Y) [26,27] or conjunction (do X *and* Y) [6]. Further, this soft optimality only bounds the deviation from simultaneously optimizing both rewards. Thus, optimizing the composition does not preclude violating safety constraints embedded in the rewards (e.g., do not enter the red tiles).

Logic Based IRL: Another promising approach for introducing compositionality has been the recent research on automata and logic based encodings of rewards [11,14] which admit well defined compositions. To this end, work has been done on inferring Linear Temporal Logic (LTL) formulas by finding the specification that minimizes the expected number of violations by an optimal agent compared to the expected number of violations by an agent applying actions uniformly at random [15]. The computation of the optimal agent's

expected violations is done via dynamic programming on the explicit product of the deterministic Rabin automaton [4] of the specification and the state dynamics. A fundamental drawback of this procedure is that due to the curse of history, it incurs a heavy run-time cost, even on simple two state and two action Markov Decision Processes. Additionally, as with early work on grammatical inference and IRL, these techniques do not produce likelihood estimates amenable to Bayesian inference.

Maximum Entropy Specification Inference: In our previous work [30], we adapted maximum entropy IRL to learn task specifications. Similar to standard maximum entropy IRL, this technique produces robust likelihood estimates. However, due to the use of the principle of maximum entropy, rather than maximum *causal* entropy, this model is limited to settings where the dynamics are deterministic or agents with open-loop policies [33].

Inference Using BDDs: This work makes heavy use of Binary Decision Diagrams (BDDs) [3] which are frequently used in symbolic value iteration for Markov Decision Processes [9] and reachability analysis for probabilistic systems [18]. However, the literature has largely relied on Multi-Terminal BDDs to encode the transition probabilities for a **single** time step. In contrast, this work introduces a two-terminal encoding based on the finite unrolling of a probabilistic circuit. To the best of our knowledge, the most similar usage of BDDs for inference appears in the independently discovered literal weight based encoding of [10] - although their encoding does not directly support non-determinism or state-indexed random variables.

Contributions: The primary contributions of this work are two fold. First, we leverage the principle of maximum causal entropy to provide the likelihood of a specification given a set of demonstrations. This formulation removes the deterministic and/or open-loop restriction imposed by prior work based on the principle of maximum entropy. Second, to mitigate the curse of history, we propose using a BDD to encode the time unrolled Markov Decision Process that the maximum causal entropy forecaster is defined over. We prove that this BDD has size that grows linearly with the horizon and quasi-linearly with the number of actions. Furthermore, we prove that our derived likelihood estimates are robust to the particular reward associated with satisfying the specification. Finally, we provide an initial experimental validation of our method. An overview of this pipeline is provided in Fig. 8.

2 Problem Setup

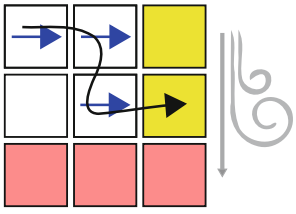
We seek to learn task specifications from demonstrations provided by a teacher who executes a sequence of actions that probabilistically change the system state. For simplicity, we assume that the set of actions and states are finite and fully observed. Further, until Sect. 5.3, we shall assume that all demonstrations are a fixed length, $\tau \in \mathbb{N}$. Formally, we begin by modeling the underlying dynamics as a probabilistic automaton.

Definition 1 *A **probabilistic automaton** (PA) is a tuple* (S, s_0, A, δ)*, where* S *is the finite set of states,* $s_0 \in S$ *is the initial state,* A *is a finite set of actions, and* δ *specifies the transition probability of going from state* s *to state* s' *given action* a*, i.e.* $\delta(s, a, s') = \Pr(s' \mid s, a)$*.*
*A **trace**[a],* ξ*, is a sequence of (action, state) pairs implicitly starting from* s_0*. A trace of length* $\tau \in \mathbb{N}$ *is an element of* $(A \times S)^\tau$*.*

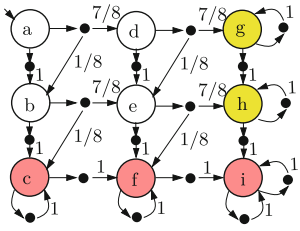
[a] *sometimes referred to as a trajectory or behavior.*

Note that probabilistic automata are equivalently characterized as *1½ player games* where each round has the agent choose an action and then the environment samples a state transition outcome. In fact, this alternative characterization is implicitly encoded in the directed bipartite graph used to visualize probabilistic automata (see Fig. 2b). In this language, we refer to the nodes where the agent makes a decision as a **decision node** and the nodes where the environment samples an outcome as a **chance node**.

Next, we develop machinery to distinguish between desirable and undesirable traces. For simplicity, we focus on finite trace properties, referred to as specifications, that are decidable within some fixed $\tau \in \mathbb{N}$ time steps, e.g., "Recharge before t = 20."



(a) Example trajectory in a gridworld where the agent can attempt to move right and down, although with a small probability the wind will move the agent down, independent of the action.



(b) PA describing the dynamics of Fig 2a as a 1½ player game. The large circles indicate states (agent decisions) and the small black circles denote the environment response probabilities.

Fig. 2. Example of gridworld probabilistic automata (PA).

Definition 2 *A **task specification**,* φ*, (or simply **specification**) is a subset of traces. For simplicity, we shall assume that each trace is of a fixed length* $\tau \in \mathbb{N}$*, e.g.,*

$$\varphi \subseteq (A \times S)^\tau \tag{1}$$

A collection of specifications, Φ*, is called a **concept class**. Further, we define* $true \stackrel{\text{def}}{=} (A \times S)^\tau$*,* $\neg\varphi \stackrel{\text{def}}{=} true \setminus \varphi$*, and* $false \stackrel{\text{def}}{=} \neg true$*.*

Often specifications are not directly given as sets, but induced by abstract descriptions of a task. For example, the task "avoid lava" induces a concrete set of traces that never enter lava tiles. If the workspace/world/dynamics change, this abstract specification would map to a different set of traces.

2.1 Specification Inference from Demonstrations

The primary task in this paper is to find the specification that best explains/-forecasts the behavior of an agent. As in our prior work [30], we formalize our problem statement as:

Definition 3 *The **specification inference from demonstrations** problem is a tuple (M, X, Φ, D) where $M = (S, s_0, A, \delta)$ is a probabilistic automaton, X is a (multi-)set of τ-length traces drawn from an unknown distribution induced by a teacher attempting to demonstrate (satisfy) some unknown task specification within M, Φ is a concept class of specifications, and D is a prior distribution over Φ. A solution to (M, X, Φ, D) is:*

$$\varphi^* \in \arg\max_{\varphi \in \Phi} \Pr(X \mid M, \varphi) \cdot \Pr_{\varphi \sim D}(\varphi) \tag{2}$$

where $\Pr(X \mid M, \varphi)$ denotes the likelihood that the teacher would have demonstrated X given the task φ.

Of course, by itself, the above formulation is ill-posed as $\Pr(X \mid M, \varphi)$ is left undefined. Below, we shall propose leveraging Maximum Causal Entropy Inverse Reinforcement Learning (IRL) to select the demonstration likelihood distribution in a regret minimizing manner.

3 Leveraging Inverse Reinforcement Learning

The key idea of Inverse Reinforcement Learning (IRL), or perhaps more accurately Inverse Optimal Control, is to find the reward structure that best explains the actions of a reward optimizing agent operating in a Markov Decision Process. We formalize below.

Definition 4 *A **Markov Decision Process (MDP)** is a probabilistic automaton endowed with a **reward map** from states to reals, $r : S \to \mathbb{R}$. This reward mapping is lifted to traces via,*

$$R(\xi) \stackrel{\text{def}}{=} \sum_{s \in \xi} r(s). \tag{3}$$

Remark 1. Note that a temporal discount factor, $\gamma \in [0, 1]$ can be added into (3) by introducing a sink state, \$, to the MDP, where $r(\$) = 0$ and

$$\Pr(s' = \$ \mid s, a) = \begin{cases} \gamma & \text{if } s \neq \$ \\ 1 & \text{otherwise} \end{cases}. \tag{4}$$

Given a MDP, the goal of an agent is to maximize the expected trace reward. In this work, we shall restrict ourselves to rewards that are given as a linear combination of **state features**, $\mathbf{f} : S \to \mathbb{R}^n_{\geq 0}$, e.g.,

$$r(s) = \theta \cdot \mathbf{f}(s) \tag{5}$$

for some $\theta \in \mathbb{R}^n$. Note that since state features can themselves be rewards, such a restriction does not actually restrict the space of possible rewards.

Example 1. Let the components of $\mathbf{f}(s)$ be distances to various locations on a map. Then the choice of θ characterizes the relative preferences in avoiding/reaching the respective locations.

Formally, we model an agent as acting according to a **policy**.

Definition 5 *A policy, π, is a state indexed distribution over actions,*

$$\Pr(a \mid s) = \pi(a \mid s). \tag{6}$$

In this language, the agent's goal is equivalent to finding a policy which maximizes the expected trace reward. We shall refer to a trace generated by such an agent as a **demonstration**. Due to the Markov requirement, the likelihood of a demonstration, ξ, given a particular policy, π, and probabilistic automaton, M, is easily stated as:

$$\Pr(\xi \mid M, \pi) = \prod_{s', a, s \in \xi} \Pr(s' \mid s, a) \cdot \Pr(a \mid s). \tag{7}$$

Thus, the likelihood of multi-set of i.i.d demonstrations, X, is given by:

$$\Pr(X \mid M, \pi) = \prod_{\xi \in X} \Pr(\xi \mid M, \pi). \tag{8}$$

3.1 Inverse Reinforcement Learning (IRL)

As previously stated, the main motivation in introducing the MDP formalism has been to discuss the inverse problem. Namely, given a set of demonstrations, find the reward that best "explains" the agent's behavior, where by "explain" one typically means that under the conjectured reward, the agent's behavior was approximately optimal. Notice however, that many undesirable rewards satisfy this property. For example, consider the following reward in which every demonstration is optimal,

$$r : s \mapsto 0. \tag{9}$$

Furthermore, observe that given a fixed reward, many policies are approximately optimal! For instance, using (9), an optimal agent could pick actions uniformly at random or select a single action to always apply.

3.2 Maximum Causal Entropy IRL

A popular, and in practice effective, solution to the lack of unique policy conundrum is to appeal to the **principle of maximum causal entropy** [32]. To formalize this principle, we recall the definitions of causally conditioned probability [17] and causal entropy [17,23].

Definition 6 *Let $X_{1:\tau} \stackrel{\text{def}}{=} X_1, \ldots, X_\tau$ denote a temporal sequence of $\tau \in \mathbb{N}$ random variables. The probability of a sequence $Y_{1:\tau}$* ***causally conditioned*** *on sequence $X_{1:\tau}$ is:*

$$\Pr(Y_{1:\tau} \mid\mid X_{1:\tau}) \stackrel{\text{def}}{=} \prod_{t=1}^{\tau} \Pr(Y_t \mid X_{1:t}, Y_{1:t-1}) \tag{10}$$

The ***causal entropy*** *of $Y_{1:\tau}$ given $X_{1:\tau}$ is defined as,*

$$H(Y_{1:\tau} \mid\mid X_{1:\tau}) \stackrel{\text{def}}{=} \mathop{\mathbb{E}}_{Y_{1:\tau}, X_{1:\tau}} [-\log(\Pr(Y_{1:\tau} \mid\mid X_{1:\tau}))] \tag{11}$$

In the case of inverse reinforcement learning, the principle of maximum causal entropy suggests forecasting using the policy whose action sequence, $A_{1:\tau}$, has the highest causal entropy, conditioned on the state sequence, $S_{1:\tau}$. That is, find the policy that maximizes

$$H(A_{1:\tau} \mid\mid S_{1:\tau}), \tag{12}$$

subject to feature matching constraints, $\mathbb{E}[\mathbf{f}]$, e.g., does the resulting policy, π^*, complete the task as seen in the data. Compared to all other policies, this policy (i) minimizes regret with respect to model/reward uncertainty, (ii) ensures that the agent's predicted policy does not depend on the future, (iii) is consistent with observed feature statistics [32].

Concretely, as proved in [32], when an agent is attempting to maximize the sum of feature state rewards, $\sum_{t=1}^{T} \theta \cdot \mathbf{f}(s_t)$, the principle of maximum causal entropy prescribes the following policy:

Maximum Causal Entropy Policy:

$$\log\left(\pi_\theta(a_t \mid s_t)\right) \stackrel{\text{def}}{=} Q_\theta(a_t, s_t) - V_\theta(s_t) \tag{13}$$

where

$$\begin{aligned} Q_\theta(a_t, s_t) &\stackrel{\text{def}}{=} \mathop{\mathbb{E}}_{s_{t+1}} [V_\theta(s_{t+1}) \mid s_t, a_t] + \theta \cdot \mathbf{f}(s_t) \\ V_\theta(s_t) &\stackrel{\text{def}}{=} \ln \sum_{a_t} e^{Q_\theta(a_t, s_t)} \stackrel{\text{def}}{=} \operatorname{softmax}_{a_t} Q_\theta(a_t, s_t). \end{aligned} \tag{14}$$

where, θ is such that (14) results in a policy which matches feature demonstrations.

Remark 2. Note that replacing softmax with max in (14) yields the standard Bellman Backup [2] used to compute the optimal policy in tabular reinforcement learning. Further, it can be shown that maximizing causal entropy corresponds to believing that the agent is exponentially biased towards high reward policies [32]:

$$\Pr(\pi_\theta \mid M) \propto \exp\Big(\mathop{\mathbb{E}}_{\xi}[R_\theta(\xi) \mid \pi_\theta, M]\Big), \tag{15}$$

where (14) is the most likely policy under (15).

Remark 3. In the special case of scalar state features, $\mathbf{f} : S \to \mathbb{R}_{\geq 0}$, the maximum causal entropy policy (14) becomes increasingly optimal as $\theta \in \mathbb{R}$ increases (since softmax monotonically approaches max). In this setting, we shall refer to θ as the agent's **rationality coefficient**.

3.3 Non-Markovian Rewards

The MDP formalism traditionally requires that the reward map be Markovian (i.e., state based); however, in practice, many tasks are history dependent, e.g. touch a red tile and then a blue tile.

A common trick within the reinforcement learning literature is to simply change the MDP and add the necessary history to the state so that the reward is Markovian, e.g. a flag for touching a red tile. However, in the case of inverse reinforcement learning, by definition, one does not know what the reward is. Therefore, one cannot assume to a priori know what history suffices.

Further exacerbating the situation is the fact that naïvely including the entire history into the state results in an exponential increase in the number of states. Nevertheless, as we shall soon see, by restricting the class of rewards to represent task specifications, this curse can be mitigated to only result in a blow-up that is at most **linear** in the state space size and in the trace length!

To this end, we shall find it fruitful to develop machinery for embedding the full trace history into the state space. Explicitly, we shall refer to the process of adding all history to a probabilistic automaton's (or MDP's) state as **unrolling**.

Definition 7 *Let $M = (S, s_0, A, \delta)$ be a PA. The **unrolling** of M is a PA, $M' = (S', s_0, A, \delta')$, where*

$$\begin{aligned} S' &= \{s_0\} \times \bigcup_{i=0}^{\infty} (A \times S)^i & \delta'(\xi_{n+1}, a, \xi_n) &= \delta(s_{n+1}, a, s_n) \\ \xi_n &= \Big(s_0, \ldots, (a_{n-1}, s_n)\Big) & \xi_{n+1} &= \Big(s_0, \ldots, (a_n, s_{n+1})\Big) \end{aligned} \tag{16}$$

If $R : S^\tau \to \mathbb{R}$ is a non-Markovian reward over τ-length traces, then we endow the corresponding unrolled PA with the now Markovian Reward,

$$r'\Big(s_0, \ldots, (a_{n-1}, s_n)\Big) \overset{\text{def}}{=} \begin{cases} R(s_0, \ldots, s_n) & \text{if } n = \tau \\ 0 & \text{otherwise} \end{cases}. \tag{17}$$

Further, by construction the reward is Markovian in S' and only depends only τ-length state sequences,

$$\sum_{t=0}^{\infty} r'\big((s_0, a_0), \dots s_\tau\big) = R(s_0, \dots, s_\tau). \tag{18}$$

Next, observe that for τ-length traces, the $1\frac{1}{2}$ player game formulation's bipartite graph forms a tree of depth τ (see Fig. 3). Further, observe that each leaf corresponds to unique τ-length trace. Thus, to each leaf, we associate the corresponding trace's reward, $R(\xi)$. We shall refer to this tree as a **decision tree**, denoted $\mathbb{T}$.

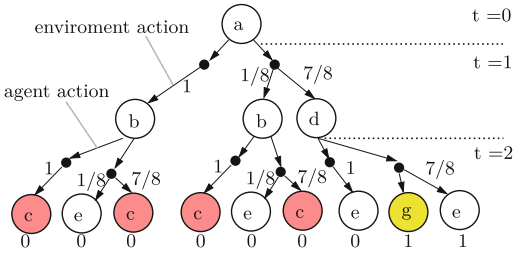


Fig. 3. Decision tree generated by the PA shown in Fig. 2 and specification "By $\tau = 2$, reach a yellow tile while avoiding red tiles.". Here a binary reward is given depending on whether or not the agent satisfies the specification. (Color figure online)

Finally, observe that the trace reward depends only on the sequence of agent actions, A, and environment actions, A_e. That is, $\mathbb{T}$ can be interpreted as a function:

$$\mathbb{T} : (A \times A_e)^\tau \to \mathbb{R}. \tag{19}$$

3.4 Specifications as Non-Markovian Rewards

Next, with the intent to frame our specification inference problem as an inverse reinforcement learning problem, we shall overload notation and denote by φ the following non-Markovian reward corresponding to a specification $\varphi \in (A \times S)^\tau$,

$$\varphi(\xi) \stackrel{\text{def}}{=} \begin{cases} 1 & \text{if } \xi \in \varphi \\ 0 & \text{otherwise} \end{cases}. \tag{20}$$

Note that the corresponding decision tree is then a Boolean predicate:

$$\mathbb{T}_\varphi : (A \times A_e)^\tau \to \{0, 1\}. \tag{21}$$

3.5 Computing Maximum Causal Entropy Specification Policies

Now let us return to the problem of computing the policy prescribed by (14). In particular, note that viewing the unrolled reward (17) as a scalar state feature results in the following soft-Bellman Backup:

$$Q_\theta(a_t, \xi_t) = \mathbb{E}\left[V_\theta(s_{t+1}) \mid \xi_t, a_t\right]$$
$$V_\theta(\xi_t) = \begin{cases} \theta \cdot \varphi(\xi_t) & \text{if } t = \tau \\ \text{softmax}_{a_t} Q_\theta(a_t, \xi_t) & \text{otherwise} \end{cases}, \tag{22}$$

where $\xi_i \in \{s_0\} \times (A \times S)^i$ denotes a state in the unrolled MDP.

Equation (22) thus suggests a naïve dynamic programming scheme over $\mathbb{T}$ starting at the $t = \tau$ leaves to compute Q_θ and V_θ (and thus π_θ).

Namely, in $\mathbb{T}$, the chance nodes, which correspond to action/state pairs, are responsible for computing Q values and the decision nodes, which correspond to states waiting for an action to be applied, are responsible for computing V values. For chance nodes this is done by taking the softmax of the values of the child nodes. Similarly, for decision nodes, this is done by taking a weighted average of the child nodes, where the weights correspond to the probability of a given transition. This, at least conceptually, corresponds to transforming $\mathbb{T}$ into a bipartite computation graph (see Fig. 4).

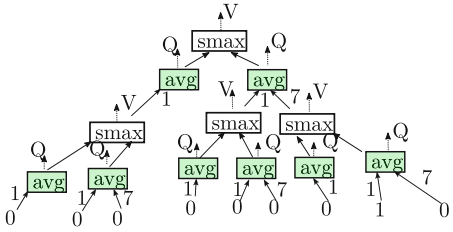


Fig. 4. Computation graph generated from applying (14) to the decision tree shown in Fig. 3. Here smax and avg denote the softmax and weighted average respectively.

Next, note that (i) the above dynamic programming scheme can be trivially modified to compute the expected trace reward of the maximum causal entropy policy and (ii) the expected reward increases[1] with the rationality coefficient θ.

Observe then that, due to monotonicity, bisection (binary search) approximates θ to tolerance ϵ in $O(\log(1/\epsilon))$ time. Additionally, notice that the likelihood of each demonstration can be computed by traversing the path of length τ in $\mathbb{T}$ corresponding to the trace and multiplying the corresponding policy and transition probabilities (8). Therefore, if $|A_e| \in \mathbb{N}$ denotes the maximum number of outcomes the environment can choose from (i.e, the branching factor for chance nodes), it follows that the run-time of this naïve scheme is:

$$O\Bigg(\overbrace{\underbrace{\left(|A| \cdot |A_e|\right)^\tau}_{|\mathbb{T}|} \cdot \underbrace{\log(1/\epsilon)}_{\text{Feature Matching}}}^{\text{compute policy}} + \underbrace{\tau|X|}_{\text{evaluate demos}}\Bigg). \tag{23}$$

[1] Formally, this is due to (a) softmax and average being monotonic (b) trajectory rewards only increasing with θ, and (c) π exponentially biasing towards high Q-values.

3.6 Task Specification Rewards

Of course, the problem with this naïve approach is that explicitly encoding the unrolled tree, $\mathbb{T}$, results in an exponential blow-up in the space and time complexity. The key insight in this paper is that the additional structure of task specifications enables avoiding such costs while still being expressive. In particular, as is exemplified in Fig. 4, the computation graphs for task specifications are often highly redundant and apt for compression.

In particular, we shall apply the following two semantic preserving transformations: (i) Eliminate nodes whose children are isomorphic sub-graphs, i.e., inconsequential decisions (ii) Combine all isomorphic sub-graphs i.e., equivalent decisions. We refer to the limit of applying these two operations as a **reduced ordered probabilistic decision diagram** and shall denote[2] the reduced variant of $\mathbb{T}$ as $\mathcal{T}$.

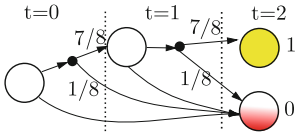


Fig. 5. Reduction of the decision tree shown in Fig. 3.

Remark 4. For those familiar, we emphasize that these decision diagrams are MDPs, not Binary Decision Diagrams (see Sect. 4). Importantly, more than two actions can be taken from a node if $\max(|A|, |A_e|) \geq 2$ and A_e has a state dependent probability distribution attached to it. That said, the above transformations are **exactly** the reduction rules for BDDs [3].

As Fig. 5 illustrates, reduced decision diagrams can be much smaller than their corresponding decision tree. Nevertheless, we shall briefly postpone characterizing $|\mathcal{T}|$ until developing some additional machinery in Sect. 4. Computationally, three problems remain.

1. How can our naïve dynamic programming scheme be adapted to this compressed structure. In particular, because many interior nodes have been eliminated, one must take care when applying (22).
2. How do concrete demonstrations map to paths in the compressed structure when evaluating likelihoods (8).
3. How can one construct $\mathcal{T}$ without first constructing $\mathbb{T}$, since failing to do so would negate any complexity savings.

We shall postpone discussing solutions to the second and third problems until Sect. 4. The first problem however, can readily be addressed with the tools at hand. Recall that in the variable ordering, nodes alternate between decision and chance nodes (i.e., agent and environment decisions), and thus alternate between taking a softmax and expectations of child values in (22). Next, by definition, if a node is skipped in $\mathcal{T}$, then it must have been inconsequential. Thus the trace reward must have been independent of the decision made at that node. Therefore, the softmax/expectation's corresponding to eliminated nodes must have been over a constant value - otherwise the eliminated sequences would

[2] Mnemonic: $\mathcal{T}$ is a (typographically) slimmed down variant of $\mathbb{T}$.

be distinguishable w.r.t φ. The result is summarized in the following identities, where α denotes the value of an eliminated node's children.

$$\text{softmax}(\overbrace{\alpha, \ldots, \alpha}^{|A|}) = \log(e^{\alpha} + \ldots + e^{\alpha}) = \ln(|A|) + \alpha \tag{24}$$

$$\mathop{\mathbb{E}}_{x}[\alpha] = \sum_{x} p(x)\alpha = \alpha \tag{25}$$

Of course, it could also be the case that a sequence of nodes is skipped in $\mathcal{T}$. Using (24), one can compute the change in value, Δ, that the eliminated sequence of n decision nodes and any number of chance nodes would have applied in $\mathbb{T}$:

$$\Delta(n, \alpha) = \ln(|A|^n) + \alpha = n \ln(|A|) + \alpha \tag{26}$$

Crucially, evaluation of this compressed computation graph is linear in $|\mathcal{T}|$ which as shall later prove, is often much smaller than $|\mathbb{T}|$.

4 Constructing and Characterizing $\mathcal{T}$

Let us now consider how to avoid the construction of $\mathbb{T}$ and characterize the size of the reduced ordered decision diagram, $\mathcal{T}$. We begin by assuming that the underlying dynamics is well-approximated in the random-bit model.

Definition 8 *For $q \in \mathbb{N}$, let $\mathbf{c} \sim \{0,1\}^q$ denote the random variable representing the result of flipping $q \in \mathbb{N}$ fair coins. We say a probabilistic automata $M = (S, s_0, A, \delta)$ is (ϵ, q) approximated in the random bit model if there exists a mapping,*

$$\hat{\delta} : S \times A \times \{0,1\}^q \to S \tag{27}$$

such that for all $s, a, s' \in S \times A \times S$:

$$\left| \delta(s, a, s') - \Pr_{\mathbf{c} \sim \{0,1\}^q} \left(\hat{\delta}(s, a, c) = s' \right) \right| \leq \epsilon. \tag{28}$$

For example, in our gridworld example (Fig. 2a), if $\mathbf{c} \in \{0,1\}^3$, elements of s are interpreted as pairs in $\mathbb{R}^2$, and the right/down actions are interpreted as the addition of the unit vectors $(1,0)$ and $(0,1)$ then,

$$\hat{\delta}(s, a, \mathbf{c}) = \begin{cases} s & \text{if } \max_i[(s+a)_i] > 1 \\ s + (0,1) & \text{else if } \mathbf{c} = 0 \\ s + a & \text{otherwise} \end{cases}, \tag{29}$$

As can be easily confirmed, (29) satisfies (28) with $\epsilon = 0$. In the sequel, we shall take access to $\hat{\delta}$ as given[3]. Further, to simplify exposition, until Sect. 5.1, we

[3] See [31] for an explanation on systematically deriving such encodings.

shall additionally require that the number of actions, $|A|$, be a power of 2. This assumption implies that A can be encoded using exactly $\log_2(|A|)$ bits.

Under the above two assumptions, the key observation is to recognize that $\mathbb{T}$ (and thus $\mathcal{T}$) can be viewed as a Boolean predicate over an alternating sequence of action bit strings and coin flip outcomes determining if the task specification is satisfied, i.e.,

$$\mathbb{T} : \{0,1\}^n \to \{0,1\}, \tag{30}$$

where $n \stackrel{\text{def}}{=} \tau \cdot \log_2(|A \times A_e|) = \tau \cdot (q + \log_2(|A|))$. That is to say, the resulting decision diagram can be re-encoded as a reduced ordered **binary** decision diagram [3].

Definition 9 *A **reduced ordered binary decision diagram** (BDD), is a representation of a Boolean predicate $h(x_1, x_2, \ldots, x_n)$ as a reduced ordered (deterministic) decision diagram, where each decision corresponds to testing a bit $x_i \in \{0,1\}$. We denote the BDD encoding of $\mathcal{T}$ as $\mathcal{B}$.*

Binary decision diagrams are well developed both in a theoretical and practical sense. Before exploring these benefits, we first note that this change has introduced an additional problem. First, note that in $\mathcal{B}$, decision and chance nodes from $\mathbb{T}$ are now encoded as sequences of decision and chance nodes. For example, if $a \in A$ is encoded by the 4-length bit sequence $b_1b_2b_3b_4$, then four decisions are made by the agent before selecting an action. Notice however that the original semantics are preserved due to associativity of the softmax and $\mathbb{E}$ operators. In particular, recall that by definition,

$$\begin{aligned} \text{softmax}(\alpha_1, \ldots, \alpha_4) &= \ln(\sum_{i=1}^{4} e^{\alpha_i}) = \ln(e^{\ln(e^{\alpha_1}+e^{\alpha_2})} + e^{\ln(e^{\alpha_3}+e^{\alpha_4})}) \\ &\stackrel{\text{def}}{=} \text{softmax}(\text{softmax}(\alpha_1, \alpha_2), \text{softmax}(\alpha_3, \alpha_4)) \end{aligned} \tag{31}$$

and thus the semantics of the sequence decision nodes is equivalent to the decision node in $\mathbb{T}$. Similarly, recall that the coin flips are fair, and thus expectations are computed via $\text{avg}(\alpha_1, \ldots, \alpha_n) = {}^1\!/_n(\sum_{i=1}^{n} \alpha_i)$. Therefore, averaging over two sequential coin flips yields,

$$\begin{aligned} \text{avg}(\alpha_1, \ldots, \alpha_4) &\stackrel{\text{def}}{=} \frac{1}{4}\sum_{i=1}^{4} \alpha_i = \frac{1}{2}(\frac{1}{2}(\alpha_1 + \alpha_2) + \frac{1}{2}(\alpha_3 + \alpha_4)) \\ &\stackrel{\text{def}}{=} \text{avg}(\text{avg}(\alpha_1, \alpha_2), \text{avg}(\alpha_3, \alpha_4)) \end{aligned} \tag{32}$$

which by assumption (28), is the same as applying $\mathbb{E}$ on the original chance node. Finally, note that skipping over decisions needs to be adjusted slightly to account for sequences of decisions. Recall that via (26), the corresponding change in value, Δ, is a function of initial value, α, and the number of agent actions skipped, i.e., $|A|^n$ for n skipped decision nodes. Thus, in the BDD, since each decision node has two actions, skipping k decision bits corresponds to skipping

2^k actions. Thus, if k decision bits are skipped over in the BDD, the change in value, Δ, becomes,

$$\Delta(k, \alpha) = \alpha + k \ln(2). \tag{33}$$

Further, note that Δ can be computed in constant time while traversing the BDD. Thus, the dynamic programming scheme is linear in the size of $\mathcal{B}$.

4.1 Size of $\mathcal{B}$

Next we return to the question of how big the compressed decision diagram can actually be. To this aim, we cite the following (conservative) bound on the size of an BDD given an encoding of the corresponding Boolean predicate in the linear model computation illustrated in Fig. 6 (for more details, we refer the reader to [16]).

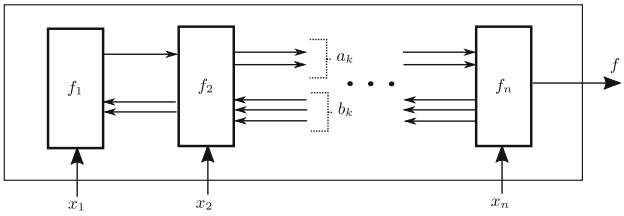


Fig. 6. Generic network of Boolean modules for which Theorem 1 holds.

In particular, consider an arbitrary Boolean predicate

$$f : \{0,1\}^n \to \{0,1\} \tag{34}$$

and a sequential arrangement of n Boolean modules, $f_1, f_2, \ldots, f_n$ where each f_i has shape:

$$f_i : \{0,1\} \times \{0,1\}^{a_{i-1}} \times \{0,1\}^{b_i} \to \{0,1\}^{a_i} \times \{0,1\}^{b_{i-1}}, \tag{35}$$

and takes as input x_i as well as a_{i-1} outputs of its left neighbor and b_i outputs of the right neighbor ($b_0 = 0, a_n = 1$). Further, assume that this arrangement is well defined, e.g. for each assignment to $x_1, \ldots, x_n$ there exists a unique way to set each of the inter-module wires. We say these modules compute f if the final output is equal to $f(x_1, \ldots, x_n)$.

Theorem 1 *If f can be computed by a linear arrangement of such modules, ordered $x_1, x_2, \ldots, x_n$, then the size, $S \in \mathbb{N}$, of its BDD (in the same order), is upper bounded [3] by:*

$$S \leq \sum_{k=1}^{n} 2^{a_k \cdot (2^{b_k})}. \tag{36}$$

To apply this bound to our problem, recall that $\mathcal{B}$ computes a Boolean function where the decisions are temporally ordered and alternate between sequences of agent and environment decisions. Next, observe that because the traces are bounded (and all finite sets are regular), there exists a finite state machine which can monitor the satisfaction of the specification.

Remark 5. In the worst case, the monitor could be the unrolled decision tree, $\mathbb{T}$. This monitor would have exponential number of states. In practice, the composition of the dynamics and the monitor is expected to be much smaller.

Further, note that because this composed system is causal, no backward wires are needed, e.g., $\forall k \;.\; b_k = 0$. In particular, observe that because the composition of the dynamics and the monitor is Markovian, the entire system can be uniquely described using the monitor/dynamics state and agent/environment action (see Fig. 7). This description can be encoded in $\log_2(2^q|A \times S \times S_\varphi|)$ bits, where q denotes the number of coin flips tossed by the environment and S_φ denotes the monitor state. Therefore, a_k is upper bounded by $\log_2(2^q|A \times S \times S_\varphi|)$. Combined with (36) this results in the following bound on the size of $\mathcal{B}$.

Corollary 1 *Let $M = (S, s_0, A, \delta)$ be a probabilistic automaton whose probabilistic transitions can be approximated using q coin flips and let φ be a specification defined for horizon τ and monitored by a finite automaton with states S_φ. The corresponding BDD, $\mathcal{B}$, has size bounded by:*

$$|\mathcal{B}| \leq \overbrace{\tau \cdot \big(\log(|A|) + q\big)}^{\#\ inputs} \cdot \overbrace{\big(2^q|A \times S \times S_\varphi|\big)}^{bound\ on\ 2^{a_k}} \tag{37}$$

Notice that the above argument implies that as the episode length grows, $|\mathcal{B}|$ grows linearly in the horizon/states and quasi-linearly in the agent/environment actions!

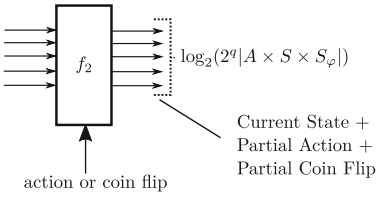


Fig. 7. Generic module in linear model of computation for $\mathcal{B}$. Note that backward edges are not required.

Remark 6. Note that this bound actually holds for the minimal representation of the composed dynamics/monitor (even if it's unknown a-prori!). For example, if the property is *true*, the BDD requires only one state (always evaluate true). This also illustrates that the above bound is often very conservative. In particular, note that for $\varphi = true$, $|\mathcal{B}| = 1$, independent of the horizon or dynamics. However, the above bound will always be linear in τ. In general, the size of the BDD will depend on the particular symmetries compressed.

Remark 7. With hindsight, Corollary 1 is not too surprising. In particular, if the monitor is known, then one could explicitly compose the dynamics MDP with the monitor, with the resulting MDP having at most $|S \times S_\varphi|$ states. If one then includes the time step in the state, one could perform the soft-Bellman

Backup directly on this automaton. In this composed automaton each (action, state) pair would need to be recorded. Thus, one would expect $O(|S \times S_\varphi \times A|)$ space to be used. In practice, this explicit representation is much bigger than $\mathcal{B}$ due to the BDDs ability to skip over time steps and automatically compress symmetries.

4.2 Constructing $\mathcal{B}$

One of the biggest benefits of the BDD representation of a Boolean function is the ability to build BDDs from a Boolean combinations of other BDDs. Namely, given two BDDs with n and m nodes respectively, it is well known that the conjunction or disjunction of the BDDs has at most $n \cdot m$ nodes. Thus, in practice, if the combined BDD's remain relatively small, Boolean combinations remain efficient to compute and one does not construct the full binary decision tree! Further, note that BDDs support function composition. Namely, given predicates $f(x_1, \ldots, x_n)$ and n predicates $g_i(y_1, \ldots, y_k)$ the function

$$f\Big(g_1(y_1, \ldots, y_k), \ldots, g_n(y_1, \ldots, y_k)\Big) \tag{38}$$

can be computed in time [16]:

$$O(n \cdot |B_f|^2 \cdot \max_i |B_{g_i}|), \tag{39}$$

where B_f is the BDD for f and B_{g_i} are the BDDs for g_i. Now, suppose $\hat{\delta}_1, \ldots \hat{\delta}_{\log(|S|)}$ are Boolean predicates such that:

$$\hat{\delta}(\mathbf{s}, \mathbf{a}, \mathbf{c}) = (\hat{\delta}_1(\mathbf{s}, \mathbf{a}, \mathbf{c}), \ldots, \hat{\delta}_{\log(|S|)}(\mathbf{s}, \mathbf{a}, \mathbf{c})). \tag{40}$$

Theorem 1 and an argument similar to that for Corollary 1 imply then that constructing $\mathcal{B}$, using repeated composition, takes time bounded by a low degree polynomial in $|A \times S \times S_\varphi|$ and the horizon. Moreover, the space complexity before and after composition are bounded by Corollary 1.

4.3 Evaluating Demonstrations

Next let us return to the question of how to evaluate the likelihood of a concrete demonstration in our compressed BDD. The key problem is that the BDD can only evaluate (binary) sequences of actions/coin flips, where as demonstrations are given as sequences of action/state pairs. That is, we need to algorithmically perform the following transformation.

$$s_0 \mathbf{a}_0 \mathbf{s}_1 \ldots \mathbf{a}_n \mathbf{s}_{n+1} \mapsto \mathbf{a}_1 \mathbf{c}_1 \ldots \mathbf{a}_n \mathbf{c}_n \tag{41}$$

Given the random bit model assumption, this transformation can be rewritten as a series of Boolean Satisfiability problems:

$$\exists\ \mathbf{c}_i\ .\ \hat{\delta}(\mathbf{s}_i, \mathbf{a}_i, \mathbf{c}_i) = \mathbf{s}_{i+1} \tag{42}$$

While potentially intimidating, in practice such problems are quite simple for modern SAT solvers, particularly if the number of coin flips used is small. Furthermore, many systems are translation invariant. In such systems, the results of a single query (42), can be reused on other queries. For example, in (29), $\mathbf{c} = \mathbf{0}$ always results in the agent moving to the right. Nevertheless, in general, if q coin flips are used, encoding all the demonstrations takes at most $O(|X| \cdot \tau \cdot 2^q)$, in the worst case.

4.4 Run-Time Analysis

We are finally ready to provide a run-time analysis for our new inference algorithm. The high-level likelihood estimation procedure is described in Fig. 8. First, the user specifies a dynamical system and a (multi-) set of demonstrations. Then, using a user-defined mechanism, a candidate task specification is selected. The system then creates a compressed representation of the composition of the dynamical system with the task specification. Then, in parallel, the maximum causal entropy policy is estimated and the demonstrations are themselves encoded as bit-vectors. Finally, the likelihood of generating the encoded demonstrations is computed.

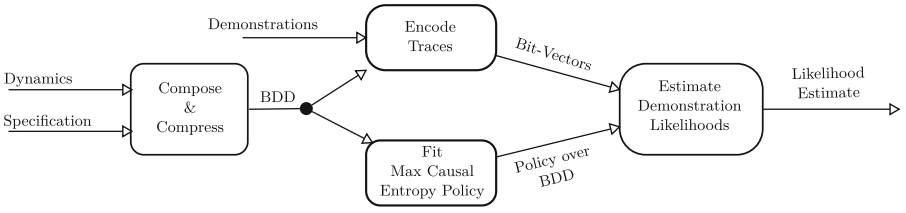


Fig. 8. High level likelihood estimation procedure described in this paper.

There are three computational bottlenecks in the compressed scheme. First, given a candidate specification, φ, one needs to construct $\mathcal{B}$. As argued in Sect. 4.2, this takes time at most polynomial in the horizon, monitoring automata size, and MDP size (in the random-bit model). Second is the process of computing Q and V values by tuning the rationality coefficient to match a particular satisfaction probability. Just as with the naïve run-time (23), this process takes time linear in the size of $|\mathcal{B}|$ and logarithmic in the inverse tolerance $1/\epsilon$. Further, using Corollary 1, we know that $|\mathcal{B}|$ is at most linear in horizon and quasi-linear in the MDP size. Thus, the policy computation takes time polynomial in the MDP size and logarithmic in the inverse tolerance. Finally, as before, evaluating the likelihoods takes time linear in the number of demonstrations and the horizon. However, we now require an additional step of finding coin-flips which are consistent with the demonstrations. Thus, the compressed run-time is bounded by:

$$O\Bigg(\Big(\underbrace{|X|}_{\#\text{Demos}} \cdot \overbrace{\log\left(\epsilon^{-1}\right)}^{\text{Feature Matching}}\Big) \cdot \text{POLY}\Big(\overbrace{\tau}^{\text{Horizon}}, \underbrace{|S|, |S_{|\varphi|}|, |A|}_{\text{Composed MDP size}}, \overbrace{2^q}^{\#\text{Coin Flip Outcomes}}\Big)\Bigg) \tag{43}$$

Remark 8. In practice, this analysis is fairly conservative since BDD composition is often fast, the bound given by Corollary 1 is loose, and the SAT queries under-consideration are often trivial.

5 Additional Model Refinements

5.1 Conditioning on Valid Actions

So far, we have assumed that the number of actions is a power of 2. Functionally, this assumption makes it so each assignment to the action decision bits corresponds to a valid action. Of course, general MDPs have non-power of 2 action sets, and so it behooves us to adapt our method for such settings. The simplest way to do so is to use a 3-terminal Binary Decision Diagram. In particular, while each decision is still Boolean, there has now three possible types of leaves, 0, 1, and $\perp$. In the adapted algorithm, edges leading to $\perp$ are simply ignored, as they semantically correspond to invalid assignments to action or coin flip bits. A similar analysis can be done using these three valued decision diagrams, and as with BDDs, there exist efficient implementations of multi-terminal BDDs.

Remark 9. This generalization also opens up the possibility of state dependent action sets, where A is now the union of all possible actions, e.g, disable the action for moving to the right when the agent is on the right edge of the grid.

5.2 Choice of Binary Co-Domain

One might wonder how sensitive this formulation is to the choice of $R(\xi) = \theta \cdot \varphi(\xi)$. In particular, how does changing the co-domain of φ from $\{0, 1\}$ to any other real values, i.e.,

$$\varphi' : (A \times S)^\tau \to \{a, b\},$$

change the likelihood estimates in our maximum causal entropy model. We briefly remark that, subject to some mild technical assumptions, almost any two real values could be used for φ's co-domain. Namely, observe that unless both a and b are zero, the expected satisfaction probability, p, is in one-to-one correspondence with the expected value of φ', i.e.,

$$\mathbb{E}[\varphi'] = a \cdot p + b \cdot (1 - p).$$

Thus, if a policy is feature matching for φ, it must be feature matching for φ' (and vice-versa). Therefore, the space of consistent policies is invariant under such transformations. Finally, because the space of policies is unchanged, the maximum causal entropy policies must remain unchanged. In practice, we prefer the use of $\{0, 1\}$ as the co-domain for φ since it often simplifies many calculations.

5.3 Variable Episode Lengths (with Discounting)

As earlier promised, we shall now discuss how to extend our model to include variable length episodes. For simplicity, we shall limit our discussion to the setting where at each time step, the probability that the episode will end is $\gamma \in (0, 1]$. As we previously discussed, this can be modeled by introducing a sink state, \$, representing the end of an episode (4). In the random bit model, this simply adds a few additional environment coin flips, corresponding to the environments new transitions to the sink state.

Remark 10. Note that when unrolled, once the end of episode transition happens, all decisions are assumed inconsequential w.r.t φ. Thus, all subsequent decisions will be compressed by in the BDD, $\mathcal{B}$.

Finally, observe that the probability that the episode ending increases exponentially, implying that the planning horizon need not be too big, i.e., the probability that the episode has not ended by timestep, $\tau \in \mathbb{N}$, is: $(1-\gamma)^\tau$. Thus, letting $\tau = \lceil \ln(\epsilon/1-\gamma) \rceil$ ensures that with probability at least $1-\epsilon$ the episode has ended.

6 Experiment

Below we report empirical results that provide evidence that our proposed technique is robust to demonstration errors and that the produced BDDs are smaller than a naïve dynamic programming scheme. To this end, we created a reference implementation [29] in Python. BDD and SAT solving capabilities are provided via dd [21] and pySAT [12] respectively. To encode the task specifications and the random-bit model MDP, we leveraged the py-aiger ecosystem [28] which includes libraries for modeling Markov Decision Processes and encoding Past Tense Temporal Logic as sequential circuits.

Problem: Consider a gridworld where an agent can attempt to move up, down, left, or right; however, with probability 1/32, the agent slips and moves left. Further, suppose a demonstrator has provided the six unlabeled demonstrations shown in Fig. 9 for the task: "Within 10 time steps, touch a yellow (recharge) tile while avoiding red (lava) tiles. Additionally, if a blue (water) tile is stepped on, the agent must step on a brown (drying) tile before going to a yellow (recharge) tile." All of the solid paths satisfy the task. The dotted path fails because the agent keeps slipping left and thus cannot dry off by $t = 10$. Note that due to slipping, all the demonstrations that did not enter the water are sub-optimal.

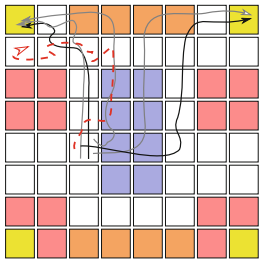


Fig. 9. Example Gridworld (Color figure online)

Spec	Policy size (#nodes)	ROBDD build time	Relative log likelihood (compared to true)
True	1	0.48s	0
φ_1 = Avoid lava	1797	1.5s	−22
φ_2 = Eventually Recharge	1628	1.2s	5
φ_3 = Don't recharge while wet	850	1.6s	−10
$\varphi_4 \stackrel{\text{def}}{=} \varphi_1 \wedge \varphi_2$	523	1.9s	4
$\varphi_5 \stackrel{\text{def}}{=} \varphi_1 \wedge \varphi_3$	1913	1.5s	−2
$\varphi_6 \stackrel{\text{def}}{=} \varphi_2 \wedge \varphi_3$	1842	2s	15
$\varphi^* \stackrel{\text{def}}{=} \varphi_1 \wedge \varphi_2 \wedge \varphi_3$	577	1.6s	27

Results: For a small collection of specifications, we have computed the size of the BDD, the time it took to construct the BDD, and the *relative* log likelihoods of the demonstrations[4],

$$\text{RelativeLogLikelihood}(\varphi) \stackrel{\text{def}}{=} \ln\left(\frac{\Pr(\text{demos} \mid \varphi)}{\Pr(\text{demos} \mid \text{true})}\right), \tag{44}$$

where each maximum entropy policy was fit to match the corresponding specification's empirical satisfaction probability. We remark that the computed BDDs are small compared to other straw-man approaches. For example, an explicit construction of the product of the monitor, dynamics, and the current time step would require space given by:

$$\tau \cdot |S| \cdot |A| \cdot |S_\varphi| = (10 \cdot 8 \cdot 8 \cdot 4) \cdot |S_\varphi| = 2560 \cdot |S_\varphi| \tag{45}$$

The resulting BDDs are much smaller than (45) and the naïve unrolled decision tree. We note that the likelihoods appear to (qualitatively) match expectations. For example, **despite** an unlabeled negative example, the demonstrated task, φ^*, is the most likely specification. Moreover, under the second most likely specification, which omits the avoid lava constraint, the sub-optimal traces that do not enter the water appear more attractive.

Finally, to emphasize the need for our causal extension, we compute the likelihoods of $\varphi^*, \varphi_1, \varphi_2$ for our opening example (Fig. 1) using both our causal model and the prior non-causal model [30]. Concretely, we take $\tau = 15$, a slip probability of 1/32, and fix the expected satisfaction probability to 0.9. The trace shown in Fig. 1 acts as the sole (failed) demonstration for φ^*. As desired, our causal extension assigned more than 3 times the relative likelihood to φ^* compared to φ_1, φ_2, and *true*. By contrast, the non-causal model assigns relative log likelihoods $(-2.83, -3.16, -3.17)$ for $(\varphi_1, \varphi_2, \varphi^*)$. This implies that (i) φ^* is the least likely specification and (ii) each specification is less likely than *true*!

[4] The maximum entropy policy for $\varphi = \text{true}$ applies actions uniformly at random.

7 Conclusion and Future Work

Motivated by the problem of learning specifications from demonstrations, we have adapted the principle of maximum causal entropy to provide a posterior probability to a candidate task specification given a multi-set of demonstrations. Further, to exploit the structure of task specifications, we proposed an algorithm that computes this likelihood by first encoding the unrolled Markov Decision Process as a reduced ordered binary decision diagram (BDD). As illustrated on a few toy examples, BDDs are often much smaller than the unrolled Markov Decision Process and thus could enable efficient computation of maximum causal entropy likelihoods, at least for well behaved dynamics and specifications.

Nevertheless, two major questions remain unaddressed by this work. First is the question of how to select which specifications to compute likelihoods for. For example, is there a way to systematically mutate a specification to make it more likely and/or is it possible to systematically reuse computations for previously evaluated specifications to propose new specifications.

Second is how to set prior probabilities. Although we have largely ignored this question, we view the problem of setting good prior probabilities as essential to avoid over fitting and/or making this technique require only one or two demonstrations. However, we note that prior probabilities can make inference arbitrarily more difficult since any structure useful for optimization imposed by our likelihood estimate can be overpowered.

Finally, additional future work includes extending the formalism to infinite horizon specifications, continuous dynamics, and characterizing the optimal set of teacher demonstrations.

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Certifying Certainty and Uncertainty in Approximate Membership Query Structures

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Abstract. Approximate Membership Query structures (AMQs) rely on randomisation for time- and space-efficiency, while introducing a possibility of false positive and false negative answers. Correctness proofs of such structures involve subtle reasoning about bounds on probabilities of getting certain outcomes. Because of these subtleties, a number of unsound arguments in such proofs have been made over the years.

In this work, we address the challenge of building rigorous and reusable computer-assisted proofs about probabilistic specifications of AMQs. We describe the framework for systematic decomposition of AMQs and their properties into a series of interfaces and reusable components. We implement our framework as a library in the Coq proof assistant and showcase it by encoding in it a number of non-trivial AMQs, such as Bloom filters, counting filters, quotient filters and blocked constructions, and mechanising the proofs of their probabilistic specifications.

We demonstrate how AMQs encoded in our framework guarantee the absence of false negatives *by construction*. We also show how the proofs about probabilities of false positives for complex AMQs can be obtained by means of *verified reduction* to the implementations of their simpler counterparts. Finally, we provide a library of domain-specific theorems and tactics that allow a high degree of automation in probabilistic proofs.

1 Introduction

Approximate Membership Query structures (AMQs) are probabilistic data structures that compactly implement (multi-)sets via hashing. They are a popular alternative to traditional collections in algorithms whose utility is not affected by some fraction of wrong answers to membership queries. Typical examples of such data structures are Bloom filters [6], quotient filters [5,38], and count-min sketches [12]. In particular, versions of Bloom filters find many applications in security and privacy [16,18,36], static program analysis [37], databases [17], web search [22], suggestion systems [45], and blockchain protocols [19,43].

Hashing-based AMQs achieve efficiency by means of losing precision when answering queries about membership of certain elements. Luckily, most of the

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applications listed above can tolerate *some* loss of precision. For instance, a static points-to analysis may consider two memory locations as aliases even if they are not (a *false positive*), still remaining sound. However, it would be unsound for such an analysis to claim that two locations do not alias in the case they do (a *false negative*). Even if it increases the number of false positives, a randomised data structure can be used to answer aliasing queries in a sound way—as long as it does not have false negatives [37]. But *how much* precision would be lost if, *e.g.*, a Bloom filter with certain parameters is chosen to answer these queries? Another example, in which quantitative properties of false positives are critical, is the security of Bitcoin's Nakamoto consensus [35] that depends on the counts of block production per unit time [19].

In the light of the described above applications, of particular interest are two kinds of properties specifying the behaviour of AMQs:

- *No-False-Negatives* properties, stating that a set-membership query for an element x always returns `true` if x is, in fact, in the set represented by the AMQ.
- Properties quantifying the rate of *False Positives* by providing a probabilistic bound on getting a wrong "yes"-answer to a membership query, given certain parameters of the data structure and the past history of its usage.

Given the importance of such claims for practical applications, it is desirable to have machine-checked formal proofs of their validity. And, since many of the existing AMQs share a common design structure, one may expect that a large portion of those validity proofs can be reused across different implementations.

Computer-assisted reasoning about the absence of *false negatives* in a particular AMQ (Bloom filter) has been addressed to some extent in the past [7]. However, to the best of our knowledge, mechanised proofs of probabilistic bounds on the *rates of false positives* did not extend to such structures. Furthermore, to the best of our knowledge, no other existing AMQs have been formally verified to date, and no attempts were made towards characterising the commonalities in their implementations in order to allow efficient proof reuse.

In this work, we aim to advance the state of the art in machine-checked proofs of probabilistic theorems about false positives in randomised hash-based data structures. As recent history demonstrates, when done in a "paper-and-pencil" way, such proofs may contain subtle mistakes [8,10] due to misinterpreted assumptions about relations between certain kinds of events. These mistakes are not surprising, as the proofs often need to perform a number complicated manipulations with expressions that capture probabilities of certain events. Our goal is to factor out these reasoning patterns into a standalone library of *reusable* program- and specification-level definitions and theorems, implemented in a proof assistant enabling computer-aided verification of a variety of AMQs.

Our Contributions. The key novel observation we make in this work is the decomposition of the common AMQ implementations into the following components: (a) a hashing strategy and (b) a state component that operates over hash outcomes, together capturing most AMQs that provide fixed constant-time insertion

and query operations. Any AMQ that is implemented as an instance of those components enjoys the *no-false-negatives* property *by construction*. Furthermore, such a decomposition streamlines the proofs of structure-specific bounds on false positive rates, while allowing for proof reuse for complex AMQ implementations, which are built on top of simpler AMQs [40]. Powered by those insights, this work makes the following technical contributions:

- A Coq-based mechanised framework Ceramist, specialised for reasoning about AMQs.[1] Implemented as a Coq library, it provides a systematic decomposition of AMQs and their properties in terms of Coq modules and uses these interfaces to to derive certain properties "for free", as well as supporting proof-by-reduction arguments between classes of similar AMQs.
- A library of non-trivial theorems for expressing closed-form probabilities on false positive rates in AMQs. In particular, we provide the first mechanised proof of the closed form for Stirling numbers of the second kind [26, Chap. 6].
- A collection of proven facts and tactics for effective construction of proofs of probabilistic properties. Our approach adopts the style of Ssreflect reasoning [21,31], and expresses its core lemmas in terms of rewrites and evaluation.
- A number of case study AMQs mechanised via Ceramist: ordinary [6] and counting [46] Bloom filters, quotient filters [5,38], and Blocked AMQs [40].

For ordinary Bloom filters, we provide the first mechanised proof that the probability of a false positive in a Bloom filter can be written as a closed form expression in terms of the input parameters; a bound that has often been mischaracterised in the past due to oversight of subtle dependencies between the components of the structure [6,34]. For Counting Bloom filters, we provide the first mechanised proofs of several of their properties: that they have no false negatives, its false positive rate, that an element can be removed without affecting queries for other elements, and the fact that Counting Bloom filters preserve the number of inserted elements irrespective of the randomness of the hash outputs. For quotient filters, we provide a mechanised proof of the false positive rate and of the absence of false negatives. Finally, alongside the standard Blocked Bloom filter [40], we derive two novel AMQ data structures: *Counting Blocked Bloom filters* and *Blocked Quotient filters*, and prove corresponding no-false-negatives and false positive rates for all of them. Our case studies illustrate that Ceramist can be repurposed to verify hash-based AMQ structures, including entirely new ones that have not been described in the literature, but rather have been obtained by composing existing AMQs via the "blocked" construction.

Our mechanised development [24] is entirely *axiom-free*, and is compatible with Coq 8.11.0 [11] and MathComp 1.10 [31]. It relies on the infotheo library [2] for encoding discrete probabilities.

Paper Outline. We start by providing the intuition on Bloom filters, our main motivating example, in Sect. 2. We proceed by explaining the encoding of their semantics, auxiliary hash-based structures, and key properties in Coq in Sect. 3.

[1] Ceramist stands for **Cer**tified **A**pproximate **M**embersh**i**p **St**ructures.

Section 4 generalises that encoding to a general AMQ interface, and provides an overview of Ceramist, its embedding into Coq, showcasing it by another example instance—Counting Bloom filters. Section 5 describes the specific techniques that help to structure our mechanised proofs. In Sect. 6, we report on the evaluation of Ceramist on various case studies, explaining in detail our compositional treatment of blocked AMQs and their properties. Section 7 provides a discussion on the state of the art in reasoning about probabilistic data structures.

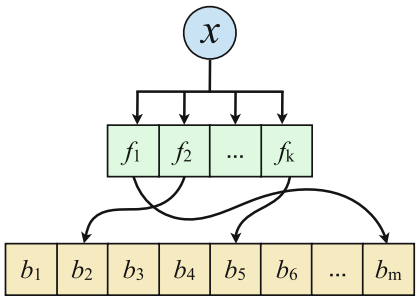
2 Motivating Example

Ceramist is a library specialised for reasoning about AMQ data structures in which the underlying randomness arises from the interaction of one or more hashing operations. To motivate this development, we thus consider applying it to the classical example of such an algorithm—a Bloom filter [6].

2.1 The Basics of Bloom Filters

Bloom filters are probabilistic data structures that provide compact encodings of mathematical sets, trading increased space efficiency for a weaker membership test [6]. Specifically, when testing membership for a value *not* in the Bloom filter, there is a possibility that the query may be answered as positive. Thus a property of direct practical importance is the exact probability of this event, and how it is influenced by the other parameters of the implementation.

A Bloom filter bf is implemented as a binary vector of m bits (all initially zeros), paired with a sequence of k hash functions $f_1, \ldots, f_k$, collectively mapping each input value to a vector of k indices from $\{1 \ldots m\}$, the indices determine the bits set to true in the m-bit array Assuming an ideal selection of hash functions, we can treat the output of $f_1, \ldots, f_k$ on new values as a uniformly-drawn random vector.



To insert a value x into the Bloom filter, we can treat each element of the "hash vector" produced from $f_1, \ldots, f_k$ as an index into bf and set the corresponding bits to ones. Similarly, to test membership for an element x, we can check that all k bits specified by the hash-vector are raised.

2.2 Properties of Bloom Filters

Given this model, there are two obvious properties of practical importance: that of false positives and of false negatives.

False Negatives. It turns out that these definitions are sufficient to guarantee the lack of false-negatives with complete certainty, *i.e.*, irrespective of the random outcome of the hash functions. This follows from the fact that once a bit is raised, there are no permitted operations that will unset it.

Theorem 1 (No False Negatives). *If* $x \in bf$*, then* $\Pr[x \in_? bf] = 1$*, where* $x \in_? bf$ *stands for the approximate membership test, while the relation* $x \in bf$ *means that* x *has been previously inserted into* bf*.*

False Positives. This property is more complex as the occurrence of a false positive is entirely dependent on the particular outcomes of the hash functions $f_1, \ldots, f_k$ and one needs to consider situations in which the hash functions happen to map some values to *overlapping* sets of indices. That is, after inserting a series of values xs, subsequent queries for $y \notin xs$ might incorrectly return `true`.

This leads to subtle dependencies that can invalidate the analysis, and have lead to a number of incorrect probabilistic bounds on the event, including in the analysis by Bloom in his original paper [6]. Specifically, Bloom first considered the probability that inserting l distinct items into the Bloom filter will set a particular bit b_i. From the independence of the hash functions, he was able to show that the probability of this event has a simple closed-form representation:

Lemma 1 (Probability of a single bit being set). *If the only values previously inserted into* bf *are* $x_1, \ldots, x_l$*, then the probability of a particular single bit at the position* i *being set is* $\Pr\left[i^{\text{th}} \text{ bit in } bf \text{ is set}\right] = 1 - \left(1 - \frac{1}{m}\right)^{kl}$.

Bloom then claimed that the probability of a false positive was simply the probability of a single bit being set, raised to the power of k, reasoning that a false positive for an element $y \notin bf$ only occurs when all the k bits corresponding to the hash outputs are set.

Unfortunately, as was later pointed out by Bose *et al.* [8], as the bits specified by $f_1(x), \ldots, f_{k-1}(x)$ may overlap, we cannot guarantee the independence that is required for any simple relation between the probabilities. Bose *et al.* rectified the analysis by instead interpreting the bits within a Bloom filter as maintaining a set $\text{bits}(bf) \subseteq \mathbb{N}_{[0,\ldots,m-1]}$, corresponding to the indices of raised bits. With this interpretation, an element y only tests positive if the random set of indices produced by the hash functions on y is such that $\text{inds}(y) \subseteq \text{bits}(bf)$. Therefore, the chance of a positive result for $y \notin bf$ resolves to the chance that the random set of indices from hashing y is a subset of the union of $\text{inds}(x)$ for each $x \in bf$. The probability of this reduced event is described by the following theorem:

Theorem 2 (Probability of False Positives). *If the only values inserted into* bf *are* $x_1, \ldots, x_l$*, then for any* $y \notin bf$*,* $\Pr[y \in_? bf] = \frac{1}{m^{k(l+1)}} \sum_{i=1}^{m} i^k i! \binom{m}{i} \left\{ {kl \atop i} \right\}$*, where* $\left\{ {s \atop t} \right\}$ *stands for the* Stirling number of the second kind*, capturing the number of surjections from a set of size* s *to a set of size* t*.*

The key step in capturing these program properties is in treating the outcomes of hashes as *random variables* and then propagating this randomness to the results of the other operations. A formal treatment of program outcomes requires a suitable semantics, representing programs as distributions of such random variables. In moving to mechanised proofs, we must first fully characterise this semantics, formally defining a notion of a probabilistic computation in Coq.

3 Encoding AMQs in Coq

To introduce our encoding of AMQs and their probabilistic behaviours in Coq, we continue with our running example, transitioning from mathematical notation to Gallina, Coq's language. The rest of this section will introduce each of the key components of this encoding through the lens of Bloom filters.

3.1 Probability Monad

Our formalisation represents probabilistic computations using an embedding following the style of the FCF library [39]. We do not use FCF directly, due to its primary focus on cryptographic proofs, wherein it provides little support for proving probabilistic bounds directly, instead prioritising a reduction-based approach of expressing arbitrary computations as compositions of known distributions.

Following the adopted FCF notation, a term of type `Comp` A represents a probabilistic computation returning a value of type A, and is constructed using the standard monadic operators, with an additional primitive `rand` n that allows sampling from a uniform distribution over the range $\mathbb{Z}_n$:

$$\begin{aligned} \texttt{ret} &: A \to \texttt{Comp}\ A \\ \texttt{bind} &: \texttt{Comp}\ A \to (A \to \texttt{Comp}\ B) \to \texttt{Comp}\ B \\ \texttt{rand} &: (n : \mathbb{N}) \to \texttt{Comp}\ (\mathbb{Z}_n) \end{aligned}$$

We implement a Haskell-style `do`-notation over this monad to allow descriptions of probabilistic computations within Gallina. For example, the following code is used to implement the query operation for the Bloom filter:

```
hash_res <-$ hash_vec_int x hashes; (* hash x using the hash functions *)
let (new_hashes, hash_vec) := hash_res in
(* check if all the corresponding bits are set *)
let qres := bf_query_int hash_vec bf in
(* return the query result and the new hashes *)
    ret (new_hashes, qres).
```

In the above listing, we pass the queried value `x` along with the hash functions `hashes` to a probabilistic hashing operation `hash_vec_int` to hash `x` over each function in `hashes`. The result of this random operation is then bound to `hash_res` and split into its constituent components—a sequence of hash outputs `hash_vec`

and an updated copy `new_hashes` of the hash functions, now incorporating the mapping for `x`. Then, having mapped our input into a sequence of indices, we can query the Bloom filter for membership using a corresponding deterministic operation `bf_query_int` to check that all the bits specified by `hash_vec` are set. Finally, we complete the computation by returning the query outcome `qres` and the updated hash functions `new_hashes` using the `ret` operation to lift our result to a probabilistic outcome.

Using the code snippet above, we can define the query operation `bf_query` as a function that maps a Bloom filter, a value to query, and a collection of hash functions to a probabilistic computation returning the query result and an updated set of hash functions. However, because our computation type does not impose any particular semantics, this result only encodes the *syntax* of the probabilistic query and has no actual meaning without a separate interpretation.

Thus, given a Gallina term of type `Comp` A, we must first evaluate it into a distribution over possible results to state properties on the probabilities of its outcomes. We interpret our monadic encoding in terms of Ramsey's probability monad [42], which decomposes a complex distribution into composition of primitive ones bound together via conditional distributions. To capture this interpretation within Coq, we then use the encoding of this monad from the infotheo library [1,2], and provide a function `eval_dist` : `Comp` $A \rightarrow$ `dist` A that evaluates computations into distributions by recursively mapping them to the probability monad. Here, `dist A` represents infotheo's encoding of distributions over a finite support `A`, defined as being composed of a measure function `pmf` : $A \rightarrow \mathbb{R}^+$, and a proof that the sum of the measure over the support A produces 1.

This mapping from computations to distributions must be done to a program e (involving, *e.g.*, Bloom filter) before stating its probability bound. Therefore, we hide this evaluation process behind a notation that allows stating probabilistic properties in a form closer to their mathematical counterparts:

$$\Pr[e = v] \triangleq (\texttt{eval\_dist}\ e)\ v$$
$$\Pr[e] \triangleq (\texttt{eval\_dist}\ e)\ \mathsf{true}$$

Above, v is an arbitrary element in the support of the distribution induced by e. Finally, we introduce a binding operator $\triangleright$ to allow concise representation of dependent distributions: $e \triangleright f \triangleq \texttt{bind}\ e\ f$.

3.2 Representing Properties of Bloom Filters

We define the state of a Bloom filter (`BF`) in Coq as a binary vector of a fixed length m, using Ssreflect's `m.-tuple` data type:

```
Record BF := mkBF { bloomfilter_state: m.-tuple bool }.
Definition bf_new : BF := (* construct a BF with all bits cleared *).
Definition bf_get_int i : BF → bool := (* retrieve BF's ith bit *).
```

We define the deterministic components of the Bloom filter implementation as pure functions taking an instance of `BF` and a series of indices assumed to be obtained from earlier calls to the associated hash functions:

$$\texttt{bf\_add\_int} : \texttt{BF} \to \texttt{seq}\ \mathbb{Z}_m \to \texttt{BF}$$
$$\texttt{bf\_query\_int} : \texttt{BF} \to \texttt{seq}\ \mathbb{Z}_m \to \texttt{bool}$$

That is, `bf_add_int` takes the Bloom filter state and a sequence of indices to insert and returns a new state with the requested bits also set. Conversely, `bf_query_int` returns `true` *iff* all the queried indices are set. These pure operations are then called within a probabilistic wrapper that handles hashing the input and the book-keeping associated with hashing to provide the standard interface for AMQs:

$$\texttt{bf\_add} : B \to (\texttt{HashVec}\ B * \texttt{BF}) \to \texttt{Comp}\ (\texttt{HashVec}\ B * \texttt{BF})$$
$$\texttt{bf\_query} : B \to (\texttt{HashVec}\ B * \texttt{BF}) \to \texttt{Comp}\ (\texttt{HashVec}\ B * \texttt{bool})$$

The component `HashVec` B (to be defined in Sect. 3.3), parameterised over an input type B, keeps track of *known results* of the involved hash functions and is provided as an external parameter to the function rather than being a part of the data structure to reflect typical uses of AMQs, wherein the hash operation is pre-determined and shared by *all* instances.

With these definitions and notation, we can now state the main theorems of interest about Bloom filters directly within Coq:[2]

Theorem 3 (No False Negatives). *For any Bloom filter state bf, a vector of hash functions hs, after having inserted an element x into bf, followed by a series xs of other inserted elements, the result of query* $x \in_? bf$ *is always* `true`*. That is, in terms of probabilities:* $\Pr\left[\texttt{bf\_add}\ x\ (hs, bf) \rhd \texttt{bf\_addm}\ xs \rhd \texttt{bf\_query}\ x\right] = 1.$

Lemma 2 (Probability of Flipping a Single Bit). *For a vector of hash functions hs of length k, after inserting a series of l distinct values xs, all unseen in hs, into an empty Bloom filter bf, represented by a vector of m bits, the probability of its any index i being set is* $\Pr\left[\texttt{bf\_addm}\ xs\ (hs, \texttt{bf\_new}) \rhd \texttt{bf\_get}\ i\right] = 1 - \left(1 - \frac{1}{m}\right)^{kl}$*. Here,* `bf_get` *is a simple embedding of the pure function* `bf_get_int` *into a probabilistic computation.*

Theorem 4 (Probability of a False Positive). *After having inserted a series of l distinct values xs, all unseen in hs, into an empty Bloom filter bf, for any unseen* $y \notin xs$*, the probability of a subsequent query* $y \in_? bf$ *for y returning* `true` *is given as* $\Pr\left[\texttt{bf\_addm}\ xs\ (hs, \texttt{bf\_new}) \rhd \texttt{bf\_query}\ y\right] = \frac{1}{m^{k(l+1)}} \sum_{i=1}^{m} i^k i! \binom{m}{i} \left\{ {kl \atop i} \right\}$.

The proof of this theorem required us to provide *the first axiom-free mechanised proof* for the closed form for Stirling numbers of the second kind [26].

In the definitions above, we used the output of the hashing operation as the bound between the deterministic and probabilistic components of the Bloom filter. For instance, in our earlier description of the Bloom filter query operation

[2] `bf_addm` is a trivial generalisation of the insertion to multiple elements.

in Sect. 3.1, we were able to implement the entire operation with the only probabilistic operation being the call `hash_vec_int x hashes`. In general, structuring AMQ operations as manipulations with hash outputs via *pure* deterministic functions allows us to decompose reasoning about the data structure into a series of specialised properties about its deterministic primitives and a separate set of reusable properties on its hash operations.

3.3 Reasoning About Hash Operations

We encode hash operations within our development using a random oracle-based implementation. In particular, in order to keep track of *seen* hashes learnt by hashing previously observed values, we represent a *state* of a hash function from elements of type `B` to a range $\mathbb{Z}_m$ using a finite map to ensure that previously hashed values produce the same hash output:

```
Definition HashState B := FixedMap B 'I_m.
```

The state is paired with a hash function generating uniformly random outputs for unseen values, and otherwise returns the value as from its prior invocations:

```
Definition hash value state : Comp (HashState B * B) :=
  match find value state with
  | Some(output) ⇒ ret (state, output)
  | None ⇒ rnd <-$ rand m;
            new_state <- put value rnd state;
            ret (new_state, rnd)
  end.
```

A *hash vector* is a generalisation of this structure to represent a vector of states of k independent hash functions:

```
Definition HashVec B := k.-tuple HashState B.
```

The corresponding hash operation over the hash vector, `hash_vec_int`, is then defined as a function taking a value and the current hash vector and then returning a pair of the updated hash vector and associated random vector, internally calling out to `hash` to compute individual hash outputs.

This random oracle-based implementation allows us to formulate several helper theorems for simplifying probabilistic computations using hashes by considering whether the hashed values *have been seen before or not*. For example, if we knew that a value x had not been seen before, we would know that the possibility of obtaining any particular choice of a vector of indices would be equivalent to obtaining the same vector by a draw from a corresponding uniform distribution. We can formalise this intuition in the form of the following theorem:

Theorem 5 (Uniform Hash Output). *For any two hash vectors hs, hs' of length k, a value x that has not been hashed before, and an output vector us of length m obtained by hashing x via hs, if the state of hs' has the same mappings*

as hs and also maps x to ıs, the probability of obtaining the pair $(hs', ıs)$ *is uniform:* $\Pr\left[\texttt{hash\_vec\_int}\ x\ hs = (hs', ıs)\right] = \left(\frac{1}{m}\right)^k$.

Similarly, there are also often cases where we are hashing a value that we *have already seen*. In these cases, if we know the exact indices a value hashes to, we can prove a certainty on the value of the outcome:

Theorem 6 (Hash Consistency). *For any hash vector hs, a value x, if hs maps x to outputs ıs, then hashing x again will certainly produce ıs and not change hs, that is,* $\Pr\left[\texttt{hash\_vec\_int}\ x\ hs = (hs, ıs)\right] = 1$.

By combining these types of probabilistic properties about hashes with the earlier Bloom filter operations, we are able to prove the prior theorems about Bloom filters by reasoning primarily about the core logical interactions of the *deterministic components* of the data structure. This decomposition is not just applicable to the case of Bloom filters, but can be extended into a general framework for obtaining modular proofs of AMQs, as we will show in the next section.

4 Ceramist at Large

Zooming out from the previous discussion of Bloom filters, we now present Ceramist in its full generality, describing the high-level design in terms of the various interfaces it requires to instantiate to obtain verified AMQ implementations.

The core of our framework revolves around the decomposition of an AMQ data structure into separate interfaces for hashing (AMQHash) and state (AMQ), generalising the specific decomposition used for Bloom filters (hash vectors and bit vectors respectively). More specifically, the AMQHash interface captures the probabilistic properties of the hashing operation, while the AMQ interface captures the deterministic interactions of the state with the hash outcomes.

4.1 AMQHash Interface

The AMQHash interface generalises the behaviours of hash vectors (Sect. 3.3) to provide a generic description of the hashing operation used in AMQs.

The interface first abstracts over the specific types used in the prior hashing operations (such as, *e.g.*, `HashVec B`) by treating them as opaque parameters: using a parameter `AMQHashState` to represent the state of the hash operation; types `Key` and `Value` encoding the hash inputs and outputs respectively, and finally, a deterministic operation `AMQHash_add_internal : AMQHashState → Key → Value → AMQHashState` to encode the interaction of the state with the outputs and inputs. For example, in the case of a single hash, the state parameter `AMQHashState` would be `HashState B`, while for a hash vector this would instead be `HashVec B`.

To use this hash state in probabilistic computations, the interface assumes a separate probabilistic operation that will take the hash state and randomly generate an output (*e.g.*, `hash` for single hashes and `hash_vec_int` for hash vectors):

```
Parameter AMQHash_hash: Key → AMQHashState → Comp (AMQHash * Value).
```

Then, to abstractly capture the kinds of reasoning about the outcomes of hash operations done with Bloom filters in Sect. 3.3, the interface assumes a few predicates on the hash state to provide information about its contents:

```
Parameter AMQHash_hashstate_contains: AMQHashState → Key → Value → bool.
Parameter AMQHash_hashstate_unseen: AMQHashState → Key → bool.
```

These components are then combined together to produce more abstract formulations of the previous Theorems 5 and 6 on hash operations.

Property 1 (Generalised Uniform Hash Output). *There exists a probability p_{hash}, such that for any two AMQ hash states hs, hs', a value x that is unseen, and an output $\imath s$ obtained by hashing x via hs, if the state of hs' has the same mappings as hs and also maps x to $\imath s$, the probability of obtaining the pair $(hs', \imath s)$ is given by:* $\Pr\left[\texttt{AMQHash\_hash}\ x\ hs = (hs', \imath s)\right] = p_{hash}$.

Property 2 (Generalised Hash Consistency). *For any AMQ hash state hs, a value x, if hs maps x to an output $\imath s$, then hashing x again will certainly produce $\imath s$ and not change hs:* $\Pr\left[\texttt{AMQhash\_hash}\ x\ hs = (hs, \imath s)\right] = 1$

Proofs of these corresponding properties must also be provided to instantiate the AMQHash interface. Conversely, components operating over this interface can assume their existence, and use them to abstractly perform the same kinds of simplifications as done with Bloom filters, resolving many probabilistic proofs to dealing with deterministic properties on the AMQ states.

4.2 The AMQ Interface

Building on top of an abstract AMQHash component, the AMQ interface then provides a unified view of the state of an AMQ and how it deterministically interacts with the output type `Value` of a particular hashing operation.

As before, the interface begins by abstracting the specific types and operations of the previous analysis of Bloom filters, first introducing a type `AMQState` to capture the state of the AMQ, and then assuming deterministic implementations of the typical *add* and *query* operations of an AMQ:

```
Parameter AMQ_add_internal: AMQState → Value → AMQState.
Parameter AMQ_query_internal: AMQState → Value → bool.
```

In the case of Bloom filters, these would be instantiated with the `BF`, `bf_add_int` and `bf_query_int` operations respectively (*cf.* Sect. 3.2), thereby setting the associated hashing operation to the hash vector (Sect. 3.3).

As we move on to reason about the behaviours of these operations, the interface diverges slightly from that of the Bloom filter by conditioning the behaviours on the assumption that the state has sufficient capacity:

```
Parameter AMQ_available_capacity: AMQState → nat → bool.
```

While the Bloom filter has no real deterministic notion of a capacity, this cannot be said of all AMQs in general, such as the Counting Bloom filter or Quotient filter, as we will discuss later.

With these definitions in hand, the behaviours of the AMQ operations are characterised using a series of associated assumptions:

Property 3 (AMQ insertion validity). *For a state s with sufficient capacity, inserting any hash output $\imath s$ into s via* `AMQ_add_internal` *will produce a new state s' for which any subsequent queries for $\imath s$ via* `AMQ_query_internal` *will return* `true`.

Property 4 (AMQ query preservation). *For any AMQ state s with sufficient remaining capacity, if queries for a particular hash output $\imath s$ in s via* `AMQ_query_internal` *happen to return* `true`*, then inserting any further outputs $\imath s'$ into s will return a state for which queries for $\imath s$ will* still *return* `true`.

Even though these assumptions seemingly place strict restrictions on the permitted operations, we found that these properties are satisfied by most common AMQ structures. One potential reason for this might be because they are in fact *sufficient* to ensure the No-False-Negatives property standard of most AMQs:

Theorem 7 (Generalised No False Negatives). *For any AMQ state s, a corresponding hash state hs, after having inserted an element x into s, followed by a series xs of other inserted elements, the result of query for x is always* `true`. *That is,* $\Pr[\texttt{AMQ\_add}\ x\ (hs, s) \rhd \texttt{AMQ\_addm}\ xs \rhd \texttt{AMQ\_query}\ x] = 1$.

Here, `AMQ_add`, `AMQ_addm`, and `AMQ_query` are generalisations of the probabilistic wrappers of Bloom filters (*cf.* Sect. 3.1) for doing the bookkeeping associated with hashing and delegating to the internal deterministic operations.

The generalised Theorem 7 illustrates one of the key facilities of our framework, wherein by simply providing components satisfying the AMQHash and AMQ interfaces, it is possible to obtain proofs of certain standard probabilistic properties or simplifications *for free*.

The diagram in Fig. 1 provides a high-level overview of the interfaces of Ceramist, their specific instances, and dependencies between them, demonstrating Ceramist's take on compositional reasoning and proof reuse. For instance Bloom filter implementation instantiates the AMQ interface implementation and uses, as a component, hash vectors, which themselves instantiate AMQHash used by AMQ. Bloom filter itself is also used as a proof reduction target by Counting Bloom filter. We will elaborate on this and the other noteworthy dependencies between interfaces and instances of Ceramist in the following sections.

4.3 Counting Bloom Filters Through Ceramist

To provide a concrete demonstration of the use of the AMQ interface, we now switch over to a new running example—Counting Bloom filters [46]. A Counting Bloom filter is a variant of the Bloom filter in which individual bits are replaced

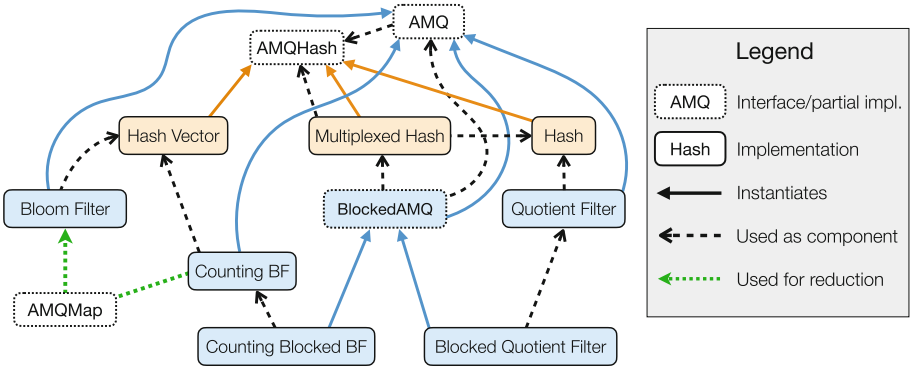


Fig. 1. Overview of Ceramist and dependencies the between its components.

with counters, thereby allowing the removal of elements. The implementation of the structure closely follows the Bloom filter, generalising the logic from bits to counters: insertion increments the counters specified by the hash outputs, while queries treat counters as set if greater than 0. In the remainder of this section, we will show how to encode and verify the Counting Bloom filter for the standard AMQ properties. We have also proven two novel domain-specific properties of Counting Bloom filters (*cf.* Appendix A of the extended paper version [25]).

First, as the Counting Bloom filter uses the same hashing strategy as the Bloom filter, the hash interface can be instantiated with the Hash Vector structure used for the Bloom filter, entirely reusing the earlier proofs on hash vectors. Next, in order to instantiate the AMQ interface, the state parameter can be defined as a vector of bounded integers, all initially set to 0:

```
Record CF := mkCF { countingbloomfilter_state: m.-tuple ℤ_p }.
Definition cf_new : CF := (* a new CF with all counters set to 0 *).
```

As mentioned before, the *add* operation increments counters rather than setting bits, and the *query* operation treats counters greater than 0 as raised.

$$\texttt{cf\_add\_int} : \texttt{CF} \to \texttt{seq}\ \mathbb{Z}_m \to \texttt{CF}$$
$$\texttt{cf\_query\_int} : \texttt{CF} \to \texttt{seq}\ \mathbb{Z}_m \to \texttt{bool}$$

To prevent integer overflows, the counters in the Counting Bloom filter are bounded to some range $\mathbb{Z}_p$, so the overall data structure too has a maximum capacity. It would not be possible to insert any values if doing such would raise any of the counters above their maximum. To account for this, the capacity parameter of the AMQ interface is instantiated with a simple predicate `cf_available_capacity` that verifies that the structure can support l further inserts by ensuring that each counter has at least $k * l$ spaces free (where k is the number of hash functions used by the data structure).

The add operation can be shown to be monotone on the value of any counter when there is sufficient capacity (Property 3). The remaining properties of the operations also trivially follow, thereby completing the instantiation, and allowing the automatic derivation of the No-False-Negatives result via Theorem 7.

4.4 Proofs About False Positive Probabilities by Reduction

As the observable behaviour of Counting Bloom filter almost exactly matches that of the Bloom filter, it seems reasonable that the same probabilistic bounds should also apply to the data structure. To facilitate these proof arguments, we provide the AMQMap interface that allows the derivation of probabilistic bounds by reducing one AMQ data structure to another.

The AMQMap interface is parameterised by two AMQ data structures, AMQ A and B, using the same hashing operation. It is assumed that corresponding bounds on False Positive rates have already been proven for AMQ B, while have not for AMQ A. The interface first assumes the existence of some mapping from the state of AMQ A to AMQ B, which satisfies a number of properties:

```
Parameter AMQ_state_map: A.AMQState → B.AMQState.
```

In the case of our Counting Bloom filter example, this mapping would convert the Counting Bloom filter state to a bit vector by mapping each counter to a raised bit if its value is greater than 0. To provide the of the false positive rate boundary, the AMQMap interface then requires the behaviour of this mapping to satisfy a number of additional assumptions:

Property 5 (AMQ Mapping Add Commutativity). *Adding a hash output to the AMQ B obtained by applying the mapping to an instance of AMQ A produces the same result as first adding a hash output to AMQ A and then applying the mapping to the result.*

Property 6 (AMQ Mapping Query Preservation). *Applying B's query operation to the result of mapping an instance of AMQ A produces the same result as applying A's query operation directly.*

In the case of reducing Counting Bloom filters (A) to Bloom filters (B), both results follow from the fact that after incrementing the some counters, all of them will have values greater than 0 and thus be mapped to raised bits.

Having instantiated the AMQMap interface with the corresponding function and proofs about it, it is now possible to derive the false positive rate of Bloom filters for Counting Bloom filters for free through the following generalised lemma:

Theorem 8 (AMQ False Positive Reduction). *For any two AMQs A, B, related by the* AMQMap *interface, if the false positive rate for B after inserting l items is given by the function f on l, then the false positive rate for A is also given by f on l. That is, in terms of probabilities:*

$$\Pr[\texttt{B.AMQ\_addm}\ xs\ (hs, \texttt{B.AMQ\_new}) \triangleright \texttt{B.AMQ\_query}\ y] = f(\texttt{length}\ xs) \implies$$
$$\Pr[\texttt{A.AMQ\_addm}\ xs\ (hs, \texttt{A.AMQ\_new}) \triangleright \texttt{A.AMQ\_query}\ y] = f(\texttt{length}\ xs).$$

5 Proof Automation for Probabilistic Sums

We have, until now, avoided discussing details of how facts about the probabilistic computations can be composed, and thereby also the specifics of how our proofs are structured. As it turns out, most of this process resolves to reasoning about summations over real values as encoded by Ssreflect's bigop library. Our development also relies on the tactic library by Martin-Dorel and Soloviev [32].

In this section, we outline some of the most essential proof principles facilitating the proofs-by-rewriting about probabilistic sums. While most of the provided rewriting primitives are standalone general equality facts, some of our proof techniques are better understood as combining a series of rewritings into a more general rewriting pattern. To delineate these two cases, will use the terminology **Pattern** to refer to a general pattern our library supports by means of a dedicated Coq tactic, while **Lemma** will refer to standalone proven equalities.

5.1 The Normal Form for Composed Probabilistic Computations

When stating properties on outcomes of a probabilistic computation (*cf.* Sect. 3.1), the computation must first be recursively evaluated into a distribution, where the intermediate results are combined using the probabilistic `bind` operator. Therefore, when decomposing a probabilistic property into smaller subproofs, we must rely on its semantics that is defined for discrete distributions as follows:

$$\texttt{bind\_dist}\ (P : \texttt{dist}\ A)\ (f : A \to \texttt{dist}\ B) \triangleq \sum_{a:\ A} \sum_{b:\ B} P\ a\ \times\ (f\ a)\ b$$

Expanding this definition, one can represent any statement on the outcome of a probabilistic computation in a *normal form* composed of only nested summations over a product of the probabilities of each intermediate computational step. This paramount transformation is captured as the following pattern:

Pattern 1 (Bind normalisation)

$$\Pr\left[(c_1 \rhd \ldots \rhd c_m) = v\right] = \sum_{v_1} \cdots \sum_{v_{m-1}} \Pr\left[c_1 = v_1\right] \times \cdots \times \Pr\left[c_m\ v_{m-1} = v\right]$$

Here, by $c_i\ v_{i-1} = v_i$, we denote the event in which the result of evaluating the command $c_i\ v_{i-1}$ is v_i, where v_{i-1} is the result of evaluating the previous command in the chain. This transformation then allows us to resolve the proof of a given probabilistic property into proving simpler statements on its substeps. For instance, consider the implementation of Bloom filter's query operation from Sect. 3.1. When proving properties of the result of a particular query (as in Theorem 3), we use this rule to decompose the program into its component parts, namely as being the product of a hash invocation $\Pr[\texttt{hash\_vec\_int}\ x\ hs]$ and the deterministic query operation `bf_query_int`. This allows dealing with the hash operation and the deterministic component *separately* by applying subsequent rewritings to each factor on the right-hand side of the above equality.

5.2 Probabilistic Summation Patterns

Having resolved a property into our normal form via a tactic implementing Pattern 1, the subsequent reductions rely on the following patterns and lemmas.

Sequential Composition. When reasoning about the properties of composite programs, it is common for some subprogram e to return a probabilistic result that is then used as the arguments for a probabilistic function f. This composition is encapsulated by the operation $e \rhd f$, as used by Theorems 3, 2, and 4. The corresponding programs, once converted to the normal form, are characterised by having factors within its internal product that simply evaluate the probability of the final statement $\texttt{ret}\ v'$ to produce a particular value v_k:

$$\sum_{v_1} \cdots \sum_{v_{m-1}} \underbrace{\Pr\left[c_1 = v_1\right] \times \cdots \Pr\left[\texttt{ret}\ v' = v_k\right]}_{e} \underbrace{\cdots \times \Pr\left[c_m\ v_{m-1} = v\right]}_{f}$$

Since the return operation is defined as a delta distribution with a peak at the return value v', we can simplify the statement by removing the summation over v_k, and replacing all occurrences of v_k with v', via the following pattern:

Pattern 2 (Probability of a Sequential Composition).

$$\begin{aligned} &\sum_{v_1} \cdots \sum_{v_{m-1}} \Pr\left[\texttt{ret}\ v' = v_1\right] \cdots \times \Pr\left[c_m\ v_{m-1} = v\right]] \\ =&\sum_{v_2} \cdots \sum_{v_{m-1}} \Pr\left[[v'/v_1](c_2\ v_1) = v_2\right] \times \cdots \times \Pr\left[[v'/v_1]c_m\ v_{m-1} = v\right] \end{aligned}$$

Notice that, without loss of generality, Pattern 2 assumes that the v'-containing factor is in the head. Our tactic implicitly rewrites the statement to this form.

Plausible Statement Sequencing. One common issue with the normal form, is that, as each statement is evaluated over the entirety of its support, some of the dependencies between statements are obscured. That is, the outputs of one statement may in fact be constrained to *some subset* of the complete support. To recover these dependencies, we provide the following theorem, that allows reducing computations under the assumption that their inputs are plausible:

Lemma 3 (Plausible Sequencing). *For any computation sequence $c_1 \rhd c_2$, if it is possible to reduce the computation $c_2\ x$ to a simpler form $c_3\ x$ when x is amongst plausible outcomes of c_1, (*i.e.*, $\Pr\left[c_1 = x\right] \neq 0$ holds) then it is possible to rewrite c_2 to c_3 without changing the resulting distribution:*

$$\sum_x \sum_y \Pr\left[c_1 = x\right] \times \Pr\left[c_2\ x = y\right] = \sum_x \sum_y \Pr\left[c_1 = x\right] \times \Pr\left[c_3\ x = y\right]$$

Plausible Outcomes. As was demonstrated in the previous paragraph, it is sometimes possible to gain knowledge that a particular value v is a plausible outcome for a composite probabilistic computation $c_1 \rhd \ldots \rhd c_m$:

$$\sum_{v_1} \cdots \sum_{v_{m-1}} \Pr\left[c_1 = v_1\right] \times \cdots \times \Pr\left[c_m\ v_{m-1} = v\right] \neq 0$$

This fact in itself is not particularly helpful as it does not immediately provide any usable constraints on the value v. However, we can now turn this inequality into a conjunction of inequalities for individual probabilities, thus getting more information about the intermediate steps of the computation:

Pattern 3. If $\sum_{v_1} \cdots \sum_{v_{m-1}} \Pr\left[c_1 = v_1\right] \times \cdots \times \Pr\left[c_m\ v_{m-1} = v\right] \neq 0$, then there exist $v_1, \ldots, v_{m-1}$ such that $\Pr\left[c_1 = v_1\right] \neq 0 \wedge \cdots \wedge \Pr\left[c_m = v\right] \neq 0$.

This transformation is possible due to the fact that probabilities are always non-negative, thus if a summation is positive, there must exist at least one element in the summation that is also positive.

Summary of the Development. By composing these components together, we obtain a comprehensive toolbox for effectively reasoning about probabilistic computations. We find that our summation patterns end up encapsulating most of the book-keeping associated with our encoding of probabilistic computations, which, combined with the AMQ/AMQHash decomposition from Sect. 4, allows for a fairly straightforward approach for verifying properties of AMQs.

5.3 A Simple Proof of Generalised No False Negatives Theorem

To showcase the fluid interaction of our proof principles in action, let us consider the proof of the generalised No-False-Negatives Theorem 7, stating the following:

$$\Pr\left[\underbrace{\texttt{AMQ\_add}\ x\ (hs, s)}_{(a),(b)} \rhd \underbrace{\texttt{AMQ\_addm}\ xs}_{(c)} \rhd \underbrace{\texttt{AMQ\_query}\ x}_{(d),(e)}\right] = 1 \tag{1}$$

As with most of our probabilistic proofs, we begin by applying normalisation Pattern 1 to reduce the computation into our normal form:

$$\sum_{\iota s_0, hs_0} \sum_{s_0} \sum_{s_1, hs_1} \sum_{\iota s_2, hs_2} \begin{pmatrix} (a)\ \Pr\left[\texttt{AMQHash\_hash}\ x\ hs = (\iota s_0, hs_0)\right] & \times \\ (b)\ \Pr\left[\texttt{ret}\ (\texttt{AMQ\_add\_internal}\ s\ \iota s_0) = s_0\right] & \times \\ (c)\ \Pr\left[\texttt{AMQ\_addm}\ xs\ (s_0, hs_0) = (s_1, hs_1)\right] & \times \\ (d)\ \Pr\left[\texttt{AMQHash\_hash}\ x\ hs_1 = (\iota s_2, hs_2)\right] & \times \\ (e)\ \Pr\left[\texttt{ret}\ (\texttt{AMQ\_query\_internal}\ s_1\ \iota s_2)\right] & \end{pmatrix}$$

We label the factors to be rewritten as (a)–(e) for the convenience of the presentation, indicating the correspondence to the components of the statement (1). From here, as all values are assumed to be unseen, we can use Property 1 in conjunction with the sequencing Pattern 2 to reduce factors (a) and (b) as follows:

$$\sum_{us_0} \sum_{s_1, hs_1} \sum_{us_2, hs_2} \begin{pmatrix} (a)\ p_{\text{hash}} & \times \\ (c)\ \Pr[\texttt{AMQ\_addm}\ xs\ ((s \leftarrow_{\text{add}} us_0), (hs \leftarrow_{\text{hash}} (x : us_0))) = (s_1, hs_1)] & \times \\ (d)\ \Pr[\texttt{AMQHash\_hash}\ x\ hs_1 = (us_2, hs_2)] & \times \\ (e)\ \Pr[\texttt{AMQ\_query\_internal}\ s_1\ us_2] & \end{pmatrix}$$

Here, p_{hash} is the probability from the statement of Property 1. We also introduce the notations $s \leftarrow_{\text{add}} us_0$ and $hs \leftarrow_{\text{hash}} (x : us_0)$ to denote the deterministic operations `AMQ_add_internal` and `AMQHash_add_internal` respectively. Then, using Pattern 3 for decomposing plausible outcomes, it is possible to separately show that any plausible hs_1 from `AMQ_addm` must map x to us_0, as hash operations preserve mappings. Combining this fact with Lemma 3 (plausible sequencing) and Hash Consistency (Property 2), we can derive that the execution of `AMQHash_hash` on x in (d) must return us_0, simplifying the summation even further:

$$\sum_{us_0} \sum_{s_1, hs_1} \begin{pmatrix} (a)\ p_{\text{hash}} & \times \\ (c)\ \Pr[\texttt{AMQ\_addm}\ xs\ ((s \leftarrow_{\text{add}} us_0), (hs \leftarrow_{\text{hash}} (x : us_0))) = (s_1, hs_1)] & \times \\ (e)\ \Pr[\texttt{AMQ\_query\_internal}\ s_1\ us_0] & \end{pmatrix}$$

Finally, as s_1 is a plausible outcome from `AMQ_addm` called on $s \leftarrow_{\text{add}} us_0$, we can then show, using Property 4 (query preservation), that querying for us_0 on s_1 must succeed. Therefore, the entire summation reduces to the summation of distributions over their support, which can be trivially shown to be 1.

6 Overview of the Development and More Case Studies

The Ceramist mechanised framework is implmented as library in Coq proof assistant [24]. It consists of three main sub-parts, each handling a different aspect of constructing and reasoning about AMQs: (i) a library of *bounded-length data structures*, enhancing MathComp's [31] support for reasoning about finite sequences with varying lengths; (ii) a library of *probabilistic computations*, extending the infotheo probability theory library [2] with definitions of deeply embedded probabilistic computations and a collection of tactics and lemmas on summations described in Sect. 5; and (iii) the *AMQ interfaces and instances* representing the core of our framework described in Sect. 4.

Alongside these core components, we also include four specific case studies to provide concrete examples of how the library can be used for practical verification. Our first two case studies are the mechanisation of the Bloom filter [6] and the Counting Bloom filter [46], as discussed earlier. In proving the false-positive rate for Bloom filters, we follow the proof by Bose *et al.* [8], also providing the first mechanised

Section	Size (LOC) Specifications	Proofs
Bounded containers	286	1051
Notation (Sect. 3.1)	77	0
Summations (Sect. 5)	742	2122
Hash operations (Sect. 4.1)	201	568
AMQ framework (Sect. 4.2)	594	695
Bloom filter (Sect. 3.2)	322	1088
Counting BF (Sect. 4.4, [25, Sect. A])	312	674
Quotient filter (Sect. 6.1)	197	633
Blocked AMQ (Sect. 6.2)	269	522

proof of the closed expression for Stirling numbers of the second kind. Our third case study provides mechanised verification of the quotient filter [5]. Our final case study is a mechanisation of the Blocked AMQ—a family of AMQs with a common aggregation strategy. We instantiate this abstract structure with each of the prior AMQs, obtaining, among others, a mechanisation of Blocked Bloom filters [40]. The sizes of each library component, along with the references to the sections that describe them, are given in the table above.

Of particular note, in effect due to the extensive proof reuse supported by Ceramist, the proof size for each of our case-studies *progressively decreases*, with around a 50% reduction in the size from our initial proofs of Bloom filters to the final case-studies of different Blocked AMQs instances.

6.1 Quotient Filter

A quotient filter [5] is a type of AMQ data structure optimised to be more cache-friendly than other typical AMQs. In contrast to the relatively simple internal vector-based states of the Bloom filters, a quotient filter works by internally maintaining a hash table to track its elements.

The internal operations of a quotient filter build upon a fundamental notion of *quotienting*, whereby a single p-bit hash outcome is split into two by treating the upper q-bits (the quotient) and the lower r-bits (the remainder) separately. Whenever an element is inserted or queried, the item is first hashed over a single hash function and then the output quotiented. The operations of the quotient filter then work by using the q-bit quotient to specify a bucket of the hash table, and the r-bit remainder as a proxy for the element, such that a query for an element will succeed if its remainder can be found in the corresponding bucket.

A false positive can occur if the outputs of the hash function happen to exactly collide for two particular values (collisions in just the quotient or remainder are not sufficient to produce an incorrect result). Therefore, it is then possible to reduce the event of a false positive in a quotient filter to the event that at least one in several draws from a uniform distribution produces a particular value. We encode quotient filters by instantiating the AMQHash interface from Sect. 4.1 with a *single* hash function, rather than a vector of hash functions, which is used by the Bloom filter variants (Sect. 2). The size of the output of this hashing operation is defined to be $2^q * 2^r$, and a corresponding quotienting operation is defined by taking the quotient and remainder from dividing the hash output by 2^q. With this encoding, we are able to provide a mechanised proof of the false positive rate for the quotient filter implemented using p-bit hash as being:

Theorem 9 (Quotient filter False Positive Rate). *For a hash-function hs, after inserting a series of l unseen distinct values xs into an empty quotient filter qf, for any unseen $y \notin xs$, the probability of a query $y \in_? qf$ for y returning* true *is given by:* $\Pr\left[\texttt{qf\_addm}\ xs\ (hs, \texttt{qf\_new}) \rhd \texttt{qf\_query}\ y\right] = 1 - \left(1 - \frac{1}{2^p}\right)^l$.

6.2 Blocked AMQ

Blocked Bloom filters [40] are a cache-efficient variant of Bloom filters where a single instance of the structure is composed of a vector of m independent Bloom filters, using an additional "meta"-hash operation to distribute values between the elements. When querying for a particular element, the meta-hash operation would first be consulted to select a particular instance to delegate the query to.

While prior research has only focused on applying this blocking design to Bloom filters, we found that this strategy is in fact generic over the choice of AMQ, allowing us to formalise an abstract Blocked AMQ structure, and later instantiate it for particular choices of "basic" AMQs. As such, this data structure highlights the scalability of Ceramist *wrt.* composition of programs and proofs.

Our encoding of Blocked AMQs within Ceramist is done via means of two higher-order modules as in Fig. 1: (*i*) a *multiplexed-hash* component, parameterised over an arbitrary hashing operation, and (*ii*) a *blocked-state* component, parameterised over some instantiation of the AMQ interface. The multiplexed hash captures the relation between the meta-hash and the hashing operations of the basic AMQ, randomly multiplexing hashes to particular hashing operations of the sub-components. We construct a multiplexed-hash as a composition of the hashing operation H used by the AMQ in each of the m blocks, and a meta-hash function to distribute queries between the m blocks. The state of this structure is defined as pairing of m states of the hashing operation H, one for each of the m blocks of the AMQ, with the state of the meta-hash function. As such, hashing a value v with this operation produces a *pair* of type $(\mathbb{Z}_m, \texttt{Value})$, where the first element is obtained by hashing v over the meta-hash to select a particular block, and the second element is produced by hashing v again over the hash operation H for this selected block. With this custom hashing operation, the state component of the Blocked AMQ is defined as sequence of m states of the AMQ, one for each block. The insertion and query operations work on the output of the multiplexed hash by using the first element to select a particular element of the sequence, and then use the second element as the value to be inserted into or queried on this selected state.

Having instantiated the data structure as described above, we proved the following abstract result about the false positive rate for blocked AMQs:

Theorem 10 (Blocked AMQ False Positive Rate). *For any AMQ A with a false positive rate after inserting l elements estimated as $f(l)$, for a multiplexed hash-function hs, after having inserted l distinct values xs, all unseen in hs, into an empty Blocked AMQ filter bf composed of m instances of A, for any unseen $y \notin xs$, the probability of a subsequent query $y \in_? bf$ for y returning* true *is given by:* $\Pr\left[\texttt{BA\_addm}\ xs\ (hs, \texttt{BA\_new}) \rhd \texttt{BA\_query}\ y\right] = \sum_{i=0}^{l} \binom{l}{i} (\frac{1}{m})^i (1 - \frac{1}{m})^{l-i} f(i)$.

We instantiated this interface with each of the previously defined AMQ structures, obtaining the Blocked Bloom filters, Counting Blocked Bloom filters and Blocked Quotient filter along with proofs of similar properties for them, for free.

7 Discussion and Related Work

Proofs About AMQs. While there has been a wealth of prior research into approximate membership query structures and their probabilistic bounds, the prevalence of paper-and-pencil proofs has meant that errors in analysis have gone unnoticed and propagated throughout the literature.

The most notable example is in Bloom's original paper [6], wherein dependencies between setting bits lead to an incorrect formulation of the bound (equation (17)), which has since been repeated in several papers [9,14,15,33] and even textbooks [34]. While this error was later identified by Bose *et al.* [8], their own analysis was also marred by an error in their definition of Stirling numbers of the second kind, resulting in yet another incorrect bound, corrected two years later by Christensen *et al.* [10], who avoided the error by eliding Stirling numbers altogether, and deriving the bound directly. Furthermore, despite these corrections, many subsequent papers [13,28–30,40,41,46] still use Bloom's original incorrect bounds. For example, in Putze *et al.* [40]'s analysis of a Blocked Bloom filter, they derive an incorrect bound on the false positive rate by assuming that the false positive of the constituent Bloom filters are given by Bloom's bound. While the Ceramist is the first development that, to the best of our knowledge, provides a mechanised proof of the probabilistic properties of Bloom filters, prior research has considered their deterministic properties. In particular, Blot *et al.* [7] provided a mechanised proof of the absence of false negatives for their implementation of a Bloom filter.

Mechanically Verified Probabilistic Algorithms. Past research has also focused on the verification of probabilistic algorithms, and our work builds on the results and ideas from several of these developments. The ALEA library tackles the task of proving properties of probabilistic algorithms [3], however in contrast to our deep embedding of computations, ALEA uses a shallow embedding through a Giry monad [20], representing probabilistic programs as measures over their outcomes. ALEA also axiomatises a custom type to represent reals between 0 and 1, which means they must independently prove any properties on reals they use, increasing the proof effort. The Foundational Cryptography Framework (FCF) [39] was developed for proving the security properties of cryptographic programs and provides an encoding of probabilistic algorithms. Rather than developing tooling for solving probabilistic obligations, their library proves probabilistic properties by reducing them to standard programs with known distributions. While this strategy follows the structure of cryptographic proofs, the simple tooling makes directly proving probabilistic bounds challenging. Tassarotti *et al.*'s Polaris [47] library for reasoning about probabilistic concurrent algorithms, also uses the same reduction strategy, and thereby inherits the same issues with proving standalone bounds. Hölzl considers mechanised verification of probabilistic programs in Isabelle/HOL [27], using a similar composition of probability and computation monads to encode probabilistic programs. However, his construction defines the semantics of programs as infinite Markov chains represented as a co-inductive streams, making it unsuitable for capturing terminating programs. Our previous

effort on mechanising the probabilistic properties of blockchains also considered the encoding of probabilistic computations in Coq [23]. While that work also relied on infotheo's probability monad, it only considered a restricted form of probabilistic properties, and did not deliver reusable tooling for the task.

Proofs of Differential Privacy. A popular motivation for reasoning about probabilistic computations is for the purposes of demonstrating differential privacy. Barthe *et al.*'s CertiPriv framework [4] extends ALEA to support reasoning using a Probabilistic Relational Hoare logic, and uses this fragment to prove probabilistic non-interference arguments. More recently, Barthe *et al.* [44] have developed a mechanisation that supports a more general coupling between distributions. Given the focus on relational properties, these developments are not suited for proving explicit numerical bounds as Ceramist is.

8 Conclusion

The key properties of Approximate Membership Query structures are inherently probabilistic. Formalisations of those properties are frequently stated incorrectly, due to the complexity of the underlying proofs. We have demonstrated the feasibility of conducting such proofs in a machine-assisted framework. The main ingredients of our approach are a principled decomposition of structure definitions and proof automation for manipulating probabilistic sums. Together, they enable scalable and reusable mechanised proofs about a wide range of AMQs.

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Global PAC Bounds for Learning Discrete Time Markov Chains

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Abstract. Learning models from observations of a system is a powerful tool with many applications. In this paper, we consider learning Discrete Time Markov Chains (DTMC), with different methods such as *frequency estimation* or *Laplace smoothing*. While models learnt with such methods converge asymptotically towards the exact system, a more practical question in the realm of trusted machine learning is how accurate a model learnt with a limited time budget is. Existing approaches provide bounds on how close the model is to the original system, in terms of bounds on *local* (transition) probabilities, which has unclear implication on the *global* behavior.

In this work, we provide *global bounds on the error* made by such a learning process, in terms of global behaviors formalized using *temporal logic*. More precisely, we propose a learning process ensuring a bound on the error in the probabilities of these properties. While such learning process cannot exist for the full LTL logic, we provide one ensuring a bound that is uniform over all the formulas of CTL. Further, given one time-to-failure property, we provide an improved learning algorithm. Interestingly, frequency estimation is sufficient for the latter, while Laplace smoothing is needed to ensure non-trivial uniform bounds for the full CTL logic.

1 Introduction

Discrete-Time Markov Chains (DTMC) are commonly used in model checking to model the behavior of stochastic systems [3,4,7,26]. A DTMC is described by a set of states and transition probabilities between these states. The main issue with modeling stochastic systems using DTMCs is to obtain the transition probabilities. One appealing approach to overcome this issue is to observe the system and to *learn automatically* these transition probabilities [8,30], e.g., using frequency estimation or Laplace (or additive) smoothing [12]. Frequency

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estimation works by observing a long run of the system and estimating each individual transition by its empirical frequency. However, in this case, the unseen transitions are estimated as zeros. Once the probability of a transition is set to zero, the probability to reach a state could be tremendously changed, e.g., from 1 to 0 if the probability of this transition in the system is small but non-zero. To overcome this problem, when the set of transitions with non-zero probability is known (but not their probabilities), Laplace smoothing assigns a positive probability to the unseen transitions, i.e., by adding a small quantity both to the numerator and the denominator of the estimate used in frequency estimation. Other smoothing methods exist, such as Good-Turing [15] and Kneser-Sey estimations [7], notably used in natural language processing. Notwithstanding smoothing generates estimation biases, all these methods converge asymptotically to the exact transition probabilities.

In practice, however, there is often limited budget in observing and learning from the system, and the validity of the learned model is in question. In trusted machine learning, it is thus crucial to measure how the learned model differs from the original system and to provide practical guidelines (e.g., on the number of observations) to guarantee some control of their divergence.

Comparing two Markov processes is a common problem that relies on a notion of divergence. Most existing approaches focus on deviations between the probabilities of local transitions (e.g., [5,10,27]). However, a single deviation in a transition probability between the original system and the learned model may lead to large differences in their global behaviors, even when no transitions are overlooked, as shown in our example 1. For instance, the probability of reaching certain state may be magnified by paths which go through the same deviated transition many times. It is thus important to use a measure that quantifies the differences over global behaviors, rather than simply checking whether the differences between the individual transition probabilities are low enough.

Technically, the knowledge of a lower bound on the transition probabilities is often assumed [1,14]. While it is a soft assumption in many cases, such as when all transition probabilities are large enough, it is less clear how to obtain such a lower bound in other cases, such as when a very unlikely transition exists (e.g., a very small error probability). We show how to handle this in several cases: learning a Markov chain accurate w.r.t. this error rate, or learning a Markov chain accurate over all its global behaviors, which is possible if we know the underlying structure of the system (e.g., because we designed it, although we do not know the precise transition probabilities which are governed by uncertain forces). For the latter, we define a new concept, namely *conditioning* of a DTMC.

In this work, we model global behaviors using temporal logics. We consider Linear Temporal Logic (LTL) [24] and Computational Tree Logic (CTL) [11]. Agreeing on all formulas of LTL means that the first order behaviors of the system and the model are the same, while agreeing on CTL means that the system and the model are bisimilar [2]. Our goal is to provide stopping rules in the learning process of DTMCs that provides Probably Approximately Correct (PAC) bounds on the error in probabilities of every property in the logic between

the model and the system. In Sect. 2, we recall useful notions on DTMCs and PAC-learning. We point out related works in Sect. 3. Our main contributions are as follows:

- In Sect. 4, we show that it is impossible to learn a DTMC accurate for all LTL formulas, by adapting a result from [13].
- We provide in Sect. 6 a learning process bounding the difference in probability *uniformly over all CTL properties*. To do so, we use Laplace smoothing, and we provide rationale on choosing the smoothing parameter.
- For the particular case of a time-to-failure property, notably used to compute the mean time between failures of critical systems (see e.g., [25]), we provide tighter bounds in Sect. 5, based on frequency estimation.

In Sect. 4, we formally state the problem and the specification that the learning process must fulfill. We also show our first contribution: the impossibility of learning a DTMC, accurate for all LTL formulas. Nevertheless, we prove in Sect. 5 our second contribution: the existence of a global bound for the time-to-failure properties, notably used to compute the mean time between failures of critical systems (see e.g., [25]) and provide an improved learning process, based on frequency estimation. In Sect. 6, we present our main contribution: a global bound guaranteeing that the original system and a model learned by Laplace smoothing have similar behaviors for all the formulas in CTL. We show that the error bound that we provide on the probabilities of properties is close to optimal. We evaluate our approach in Sect. 7 and conclude in Sect. 8.

2 Background

In this section, we introduce the notions and notations used throughout the paper. A stochastic system $\mathcal{S}$ is interpreted as a set of interacting components in which the state is determined randomly with respect to a global probability measure described below.

Definition 1 (Discrete-Time Markov Chains). *A Discrete-Time Markov Chain is a triple* $\mathcal{M} = (S, \mu, A)$ *where:*

- S *is a finite set of states;*
- $\mu : S \to [0, 1]$ *is an initial probability distribution over* S*;*
- $A : S \times S \to [0, 1]$ *is a transition probability matrix, such that for every* $s \in S$, $\sum_{s' \in S} A(s, s') = 1$.

We denote by m the cardinal of S and $A = (a_{ij})_{1 \leq i,j \leq m} = (A(i, j))_{1 \leq i,j \leq m}$ the probability matrix. Figures 1 and 2 show the graph of two DTMCs over 3 states $\{s_1, s_2, s_3\}$ (with $\mu(s_1) = 1$). A run is an infinite sequence $\omega = s_0 s_1 \cdots$ and a path is a finite sequence $\omega = s_0 \cdots s_l$ such that $\mu(s_0) > 0$ and $A(s_i, s_{i+1}) > 0$ for all i, $0 \leq i \leq l$. The length $|\omega|$ of a path ω is its number of transitions.

The cylinder set of ω, denoted $C(\omega)$, consists of all the runs starting by a path ω. Markov chain $\mathcal{M}$ underlies a probability space $(\Omega, \mathcal{F}, \mathbb{P})$, where Ω is the

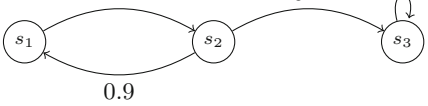

Fig. 1. An example of DTMC $\mathcal{M}_1$

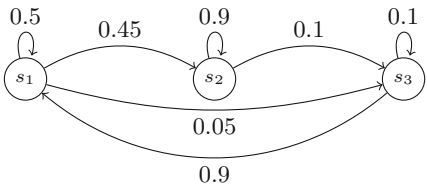

Fig. 2. DTMC $\mathcal{M}_2$

set of all runs from $\mathcal{M}$; $\mathcal{F}$ is the sigma-algebra generated by all the cylinders $C(\omega)$ and $\mathbb{P}$ is the unique probability measure [32] such that $\mathbb{P}(C(s_0 \cdots s_l)) = \mu(s_0) \prod_{i=1}^{l} A(s_{i-1}, s_i)$. For simplicity, we assume a unique initial state s_0 and denote $\mathbb{P}(\omega) = \mathbb{P}(C(\omega))$. Finally, we sometimes use the notation $\mathbb{P}_i^A$ to emphasize that the probability distribution is parameterized by the probability matrix A, and the starting state is i.

2.1 PAC-Learning for Properties

To analyze the behavior of a system, properties are specified in temporal logic (e.g., LTL or CTL, respectively introduced in [24] and [11]). Given a logic $\mathcal{L}$ and φ a property of $\mathcal{L}$, decidable in finite time, we denote $\omega \models \varphi$ if a path ω satisfies φ. Let $z : \Omega \times \mathcal{L} \to \{0, 1\}$ be the function that assigns 1 to a path ω if $\omega \models \varphi$ and 0 otherwise. In what follows, we assume that we have a procedure that draws path ω with respect to $\mathbb{P}^A$ and outputs $z(\omega, \varphi)$. Further, we denote $\gamma(A, \varphi)$ the probability that a path drawn with respect to $\mathbb{P}^A$ satisfies φ. We omit the property or the matrix in the notation when it is clear from the context. Finally, note that the behavior of $z(., \varphi)$ can be modeled as a Bernoulli random variable Z_φ parameterized by the mean value $\gamma(A, \varphi)$.

Probably Approximately Correct (PAC) learning [28] is a framework for mathematical analysis of machine learning. Given $\varepsilon > 0$ and $0 < \delta < 1$, we say that a property φ of $\mathcal{L}$ is PAC-learnable if there is an algorithm $\mathcal{A}$ such that, given a sample of n paths drawn according to the procedure, with probability of at least $1-\delta$, $\mathcal{A}$ outputs in polynomial time (in $1/\varepsilon$ and $1/\delta$) an approximation of the average value for Z_φ close to its exact value, up to an error less than or equal to ε. Formally, φ is PAC-learnable if and only if $\mathcal{A}$ outputs an approximation $\hat{\gamma}$ such that:

$$\mathbb{P}(|\gamma - \hat{\gamma}| > \varepsilon) \leq \delta \tag{1}$$

Moreover, if the above statement for algorithm $\mathcal{A}$ is true for every property in $\mathcal{L}$, we say that $\mathcal{A}$ is a PAC-learning algorithm for $\mathcal{L}$.

2.2 Monte-Carlo Estimation and Algorithm of Chen

Given a sample W of n paths drawn according to $\mathbb{P}^A$ until φ is satisfied or violated (for φ such that with probability 1, φ is eventually satisfied or violated), the crude Monte-Carlo estimator, denoted $\hat{\gamma}_W(A, \varphi)$, of the mean value

for the random variable Z_φ is given by the empirical frequency: $\hat{\gamma}_W(A,\varphi) = \frac{1}{n}\sum_{i=1}^{n} z(\omega_i) \approx \gamma(A,\varphi)$.

The Okamoto inequality [23] (also called the Chernoff bound in the literature) is often used to guarantee that the deviation between a Monte-Carlo estimator $\hat{\gamma}_W$ and the exact value γ by more than $\varepsilon > 0$ is bounded by a predefined confidence parameter δ. However, several sequential algorithms have been recently proposed to guarantee the same confidence and accuracy with fewer samples[1]. In what follows, we use the Massart bound [22], implemented in the algorithm of Chen [6].

Theorem 1 (Chen bound). *Let $\varepsilon > 0$, δ such that $0 < \delta < 1$ and $\hat{\gamma}_W$ be the crude Monte-Carlo estimator, based on n samples, of probability γ.*

If $n \geq \frac{2}{\varepsilon^2}\log\left(\frac{2}{\delta}\right)\left[\frac{1}{4} - (|\frac{1}{2} - \hat{\gamma}_W| - \frac{2}{3}\varepsilon)^2\right]$,

$$\mathbb{P}(|\gamma - \hat{\gamma}_W| > \varepsilon) \leq \delta.$$

To ease the readability, we write $n_{\text{succ}} = \sum_{i=1}^{n} z(\omega_i)$ and $H(n, n_{\text{succ}}, \epsilon, \delta) = \frac{2}{\varepsilon^2}\log\left(\frac{2}{\delta}\right)\left[\frac{1}{4} - (|\frac{1}{2} - \hat{\gamma}_W| - \frac{2}{3}\varepsilon)^2\right]$. When it is clear from the context, we only write $H(n)$. Then, the algorithm $\mathcal{A}$ that stops sampling as soon as $n \geq H(n)$ and outputs a crude Monte-Carlo estimator for $\gamma(A,\varphi)$ is a PAC-learning algorithm for φ. The condition over n is called the stopping criteria of the algorithm. As far as we know, this algorithm requires fewer samples than the other sequential algorithms (see e.g., [18]). Note that the estimation of a probability close to $1/2$ likely requires more samples since $H(n)$ is maximized in $\hat{\gamma}_W = 1/2$.

3 Related Work

Our work shares similar statistical results (see Sect. 2.3) with Statistical Model Checking (SMC) [32]. However, the context and the outputs are different. SMC is a simulation-based approach that aims to estimate one probability for a given property [9,29], within acceptable margins of error and confidence [17,18,33]. A challenge in SMC is posed by unbounded properties (e.g., fairness) since the sampled executions are finite. Some algorithms have been proposed to handle unbounded properties but they require the knowledge of the minimal probability transition of the system [1,14], which we avoid. While this restriction is light in many contexts, such as when every state and transition appears with a sufficiently high probability, contexts where probabilities are unknown and some are very small seems much harder to handle. In the following, we propose 2 solutions not requiring this assumption. The first one is the closest to SMC: we learn a Markov chain accurate for a given time-to-error property, and it does not require knowledge on the Markov chain. The second one is much more ambitious than SMC as it learns a Markov chain accurate for *all* its global behaviors, formalized as all properties of a temporal logic; it needs the assumption that the set

[1] We recall the Okamoto-Chernoff bound in the extended version (as well as the Massart bound), but we do not use it in this work.

of transitions is known, but not their probabilities nor a lower bound on them. This assumption may seem heavy, but it is reasonable for designers of systems, for which (a lower bound on) transition probabilities are not known (e.g. some error rate of components, etc).

For comparison with SMC, our final output is the (approximated) transition matrix of a DTMC rather than one (approximated) probability of a given property. This learned DTMC can be used for different purposes, e.g. as a component in a bigger model or as a simulation tool. In terms of performances, we will show that we can learn a DTMC w.r.t. a given property with the same number of samples as we need to estimate this property using SMC (see Sect. 5). That is, there is no penalty to estimate a DTMC rather than estimate one probability, and we can scale as well as SMC. In terms of expressivity, we can handle unbounded properties (e.g. fairness properties). Even better, we can learn a DTMC accurate uniformly over a possibly infinite set of properties, e.g. all formulas of CTL. This is something SMC is not designed to achieve.

Other related work can be cited: In [13], the authors investigate several distances for the estimation of the difference between DTMCs. But they do not propose algorithms for learning. In [16], the authors propose to analyze the learned model a posteriori to test whether it has some good properties. If not, then they tweak the model in order to enforce these properties. Also, several PAC-learning algorithms have been proposed for the estimation of stochastic systems [5,10] but these works focus on local transitions instead of global properties.

4 Problem Statement

In this work, we are interested to learn a DTMC model from a stochastic system $\mathcal{S}$ such that the behaviors of the system and the model are similar. We assume that the original system is a DTMC parameterized by a matrix A of transition probabilities. The transition probabilities are unknown, but the set of states of the DTMC is assumed to be known.

Our goal is to provide a learning algorithm $\mathcal{A}$ that guarantees an accurate estimation of $\mathcal{S}$ with respect to certain global properties. For that, a sampling process is defined as follows. A path (i.e., a sequence of states from s_0) of $\mathcal{S}$ is observed, and at steps specified by the sampling process, a reset action is performed, setting $\mathcal{S}$ back to its initial state s_0. Then another path is generated. This process generates a set W of paths, called traces, used to learn a matrix $\hat{A}_W$. Formally, we want to provide a learning algorithm that guarantees the following specification:

$$\mathbb{P}(\mathcal{D}(A, \hat{A}_W) > \varepsilon) \leq \delta \tag{2}$$

where $\varepsilon > 0$ and $\delta > 0$ are respectively *accuracy* and *confidence* parameters and $\mathcal{D}(A, \hat{A}_W)$ is a measure of the divergence between A and $\hat{A}_W$.

There exist several ways to specify the divergence between two transition matrices, e.g., the Kullback-Leibler divergence [19] or a distance based on a matrix norm. However, the existing notions remain heuristic because they are

based on the difference between the individual probabilistic transitions of the matrix. We argue that what matters in practice is often to quantify the similarity between the global behaviors of the systems and the learned model.

In order to specify the behaviors of interest, we use a property φ or a set of properties Ψ on the set of states visited. We are interested in the difference between the probabilities of φ (i.e., the measure of the set of runs satisfying φ) with respect to A and $\hat{A}_W$. We want to ensure that this difference is less than some predefined ε with (high) probability $1 - \delta$. Hence, we define:

$$\mathcal{D}_\varphi(A, \hat{A}_W) = |\gamma(A, \varphi) - \gamma(\hat{A}_W, \varphi)| \tag{3}$$

$$\mathcal{D}_\Psi(A, \hat{A}_W) = \max_{\varphi \in \Psi}(\mathcal{D}_\varphi(A, \hat{A}_W)) \tag{4}$$

Our problem is to construct an algorithm which takes the following as inputs:

- confidence δ, $0 < \delta < 1$,
- absolute error $\varepsilon > 0$, and
- a property φ (or a set of properties Ψ),

and provides a learning procedure sampling a set W of paths, outputs $\hat{A}_W$, and terminates the sampling procedure while fulfilling Specification (2), with $\mathcal{D} = \mathcal{D}_\varphi$ $(= \mathcal{D}_\Psi)$.

In what follows, we assume that the confidence level δ and absolute error ε are fixed. We first start with a negative result: if Ψ is the set of LTL formulas [2], such a learning process is impossible.

Theorem 2. *Given $\varepsilon > 0$, $0 < \delta < 1$, and a finite set W of paths randomly drawn with respect to a DTMC A, there is no learning strategy such that, for every LTL formula φ,*

$$\mathbb{P}(|\gamma(A, \varphi) - \gamma(\hat{A}_W, \varphi)| > \varepsilon) \leq \delta \tag{5}$$

Note that contrary to Theorem 1, the deviation in Theorem 2 is a difference between two exact probabilities (of the original system and of a learned model). The theorem holds as long as $\hat{A}_W$ and A are not strictly equal, no matter how $\hat{A}_W$ is learned. To prove this theorem, we show that, for any number of observations, we can always define a sequence of LTL properties that violates the specification above. It only exploits a single deviation in one transition. The proof, inspired by a result from [13], is given in the extended version.

Example 1. We show in this example that in general, one needs to have some knowledge on the system in order to perform PAC learning - either a positive lower bound $\ell > 0$ on the lowest probability transition, as in [1,14], or the support of transitions (but no knowledge on their probabilities), as we use in Sect. 6. Further, we show that the latter assumption does not imply the former, as even if no transitions are overlooked, the error in some reachability property can be arbitrarily close to 0.5 even with arbitrarily small error on the transition probabilities.

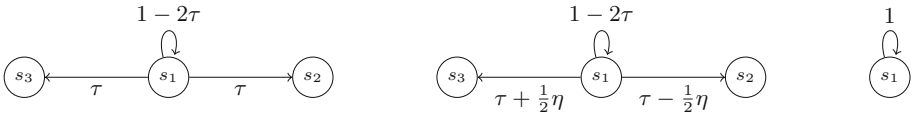

Fig. 3. Three DTMCs $A, \hat{A}, \hat{B}$ (from left to right), with $0 < \eta < 2\tau < 1$

Let us consider DTMCs $A, \hat{A}, \hat{B}$ in Fig. 3, and formula $\mathbf{F}\, s_2$ stating that s_2 is eventually reached. The probabilities to satisfy this formula in $A, \hat{A}, \hat{B}$ are respectively $\mathbb{P}^A(\mathbf{F}\, s_2) = \frac{1}{2}$, $\mathbb{P}^{\hat{A}}(\mathbf{F}\, s_2) = \frac{2\tau-\eta}{4\tau} = \frac{1}{2} - \frac{\eta}{4\tau}$ and $\mathbb{P}^{\hat{B}}(\mathbf{F}\, s_2) = 0$.

Assume that A is the real system and that $\hat{A}$ and $\hat{B}$ are DTMCs we learned from A. Obviously, one wants to avoid learning $\hat{B}$ from A, as the probability of $\mathbf{F}\, s_2$ is very different in $\hat{B}$ and in $\hat{A}$ (0 instead of 0.5). If one knows that $\tau > \ell$ for some lower bound $\ell > 0$, then one can generate enough samples from s_1 to evaluate τ with an arbitrarily small error $\frac{\eta}{2} << \ell$ on probability transitions with an arbitrarily high confidence, and in particular learn a DTMC similar to $\hat{A}$.

On the other hand, if one knows there are transitions from s_1 to s_2 and to s_3, then immediately, one does not learn DTMC $\hat{B}$, but a DTMC similar to DTMC $\hat{A}$ (using e.g. Laplace smoothing [12]). While this part is straightforward with this assumption, evaluating τ is much harder when one does not know a priori a lower bound $\ell > 0$ such that $\tau > \ell$. That is very important: while one can make sure that the error $\frac{\eta}{2}$ on probability transitions is arbitrarily small, if τ is unknown, then it could be the case that τ is as small as $\frac{\eta}{2(1-\varepsilon)} > \frac{\eta}{2}$, for a small $\varepsilon > 0$. This gives us $\mathbb{P}^{\hat{A}}(\mathbf{F}\, s_2) = \frac{1}{2} - \frac{1-\varepsilon}{2} = \frac{\varepsilon}{2}$, which is arbitrarily small, whereas $\mathbb{P}^A(\mathbf{F}\, s_2) = 0.5$, leading to a huge error in the probability to reach s_2. We work around that problem in Sect. 6 by defining and computing the *conditioning* of DTMC $\hat{A}$. In some particular cases, as the one discussed in the next section, one can avoid that altogether (actually, the conditioning in these cases is perfect (=1), and it needs not be computed explicitly).

5 Learning for a Time-to-failure Property

In this section, we focus on property φ of reaching a failure state s_F from an initial state s_0 without re-passing by the initial state, which is often used for assessing the failure rate of a system and the mean time between failures (see e.g., [25]). We assume that with probability 1, the runs eventually re-pass by s_0 or reach s_F. Also, without loss of generality, we assume that there is a unique failure state s_F in A. We denote $\gamma(A, \varphi)$ the probability, given DTMC A, of satisfying property φ, i.e., the probability of a failure between two visits of s_0.

Assume that the stochastic system $\mathcal{S}$ is observed from state s_0. Between two visits of s_0, property φ can be monitored. If s_F is observed between two instances of s_0, we say that the path $\omega = s_0 \cdot \rho \cdot s_F$ satisfies φ, with $s_0, s_F \notin \rho$. Otherwise, if s_0 is visited again from s_0, then we say that the path $\omega = s_0 \cdot \rho \cdot s_0$ violates φ, with $s_0, s_F \notin \rho$. We call *traces* paths of the form $\omega = s_0 \cdot \rho \cdot (s_0 \vee s_F)$

with $s_0, s_F \notin \rho$. In the following, we show that it is sufficient to use a *frequency estimator* to learn a DTMC which provides a good approximation for such a property.

5.1 Frequency Estimation of a DTMC

Given a set W of n traces, we denote n_{ij}^W the number of times a transition from state i to state j has occurred and n_i^W the number of times a transition has been taken from state i.

The *frequency estimator* of A is the DTMC $\hat{A}_W = (\hat{a}_{ij})_{1 \leq i,j \leq m}$ given by $\hat{a}_{ij} = \frac{n_{ij}^W}{n_i^W}$ for all i, j, with $\sum_{i=1}^m n_i^W = \sum_{i=1}^m \sum_{j=1}^m n_{ij}^W = |W|$. In other words, to learn $\hat{A}_W$, it suffices to count the number of times a transition from i to j occurred, and divide by the number of times state i has been observed. The matrix $\hat{A}_W$ is trivially a DTMC, except for states i which have not been visited. In this case, one can set $\hat{a}_{ij} = \frac{1}{m}$ for all states j and obtain a DTMC. This has no impact on the behavior of $\hat{A}_W$ as i is not reachable from s_0 in $\hat{A}_W$.

Let $\hat{A}_W$ be the matrix learned using the frequency estimator from the set W of traces, and let A be the real probabilistic matrix of the original system $\mathcal{S}$. We show that, in the case of time-to-failure properties, $\gamma(\hat{A}_W, \varphi)$ is equal to the crude Monte Carlo estimator $\hat{\gamma}_W(A, \varphi)$ induced by W.

5.2 PAC Bounds for a Time-to-failure Property

We start by stating the main result of this section, bounding the error between $\gamma(A, \varphi)$ and $\gamma(\hat{A}_W, \varphi)$:

Theorem 3. *Given a set W of n traces such that $n = \lceil H(n) \rceil$, we have:*

$$\mathbb{P}\left(|\gamma(A, \varphi) - \gamma(\hat{A}_W, \varphi)| > \varepsilon\right) \leq \delta \tag{6}$$

where $\hat{A}_W$ is the frequency estimator of A.

To prove Theorem (3), we first invoke Theorem 1 to establish:

$$\mathbb{P}\left(|\gamma(A, \varphi) - \hat{\gamma}_W(A, \varphi)| > \varepsilon\right) \leq \delta \tag{7}$$

It remains to show that $\hat{\gamma}_W(A, \varphi) = \gamma(\hat{A}_W, \varphi)$:

Proposition 1. *Given a set W of traces, $\gamma(\hat{A}_W, \varphi) = \hat{\gamma}_W(A, \varphi)$.*

It might be appealing to think that this result can be proved by induction on the size of the traces, mimicking the proof of computation of reachability probabilities by linear programming [2]. This is actually not the case. The remaining of this section is devoted to proving Proposition (1).

We first define $q_W(u)$ the number of occurrences of sequence u in the traces of W. Note that u can be a state, an individual transition or even a path. We also use the following definitions in the proof.

Definition 2 (Equivalence). *Two sets of traces W and W' are equivalent if for all $s,t \in S$, $\frac{q_W(s\cdot t)}{q_W(s)} = \frac{q_{W'}(s\cdot t)}{q_{W'}(s)}$.*

We define a set of traces W' equivalent with W, implying that $\hat{A}_W = \hat{A}_{W'}$. This set W' of traces satisfies the following:

Lemma 1. *For any set of traces W, there exists a set of traces W' such that:*

(i) W and W' are equivalent,

(ii) for all $r,s,t \in S$, $q_{W'}(r\cdot s\cdot t) = \dfrac{q_{W'}(r\cdot s)\times q_{W'}(s\cdot t)}{q_{W'}(s)}$.

The proof of Lemma 1 is provided in the extended version. In Lemma 1, (i) ensures that $\hat{A}_{W'} = \hat{A}_W$ and (ii) ensures the equality between the proportion of runs of W' passing by s and satisfying γ, denoted $\hat{\gamma}^s_{W'}$, and the probability of reaching s_F before s_0 starting from s with respect to $\hat{A}_{W'}$. Formally,

Lemma 2. *For all $s \in S$, $\mathbb{P}_s^{\hat{A}_{W'}}(\text{reach } s_f \text{ before } s_0) = \hat{\gamma}^s_{W'}$.*

Proof. Let S_0 be the set of states s with no path in $\hat{A}_{W'}$ from s to s_f without passing through s_0. For all $s \in S_0$, let $p_s = 0$. Also, let $p_{s_f} = 1$. Let $S_1 = S\setminus(S_0 \cup \{s_f\})$. Consider the system of Eq. (8) with variables $(p_s)_{s\in S_1} \in [0,1]^{|S_1|}$:

$$\forall\, s \in S_1, \quad p_s = \sum_{t=1}^{m} \hat{A}_{W'}(s,t)p_t \tag{8}$$

The system of Eq. (8) admits a unique solution according to [2] (Theorem 10.19. page 766). Then, $(\mathbb{P}_s^{\hat{A}_{W'}}(\text{reach } s_f \text{ before } s_0))_{s\in S_1}$ is trivially a solution of (8). But, since W' satisfies the conditions of Lemma 1, we also have that $(\hat{\gamma}^s_{W'})_{s\in S_1}$ is a solution of (8), and thus we have the desired equality. □

Notice that Lemma 2 does not hold in general with the set W. We have:

$$\begin{aligned}
\hat{\gamma}_W(A,\varphi) &= \hat{\gamma}^{s_0}_W \quad \text{(by definition)}\\
&= \hat{\gamma}^{s_0}_{W'} \quad \text{(by Lemma 1)}\\
&= \mathbb{P}_{s_0}^{\hat{A}_{W'}}(\text{reach } s_f \text{ before } s_0) \quad \text{(by Lemma 2)}\\
&= \mathbb{P}_{s_0}^{\hat{A}_W}(\text{reach } s_f \text{ before } s_0) \quad \text{(by Lemma 1)}\\
&= \gamma(\hat{A}_W,\varphi) \quad \text{(by definition).}
\end{aligned}$$

That concludes the proof of Proposition 1. It shows that learning can be as efficient as statistical model-checking on comparable properties.

6 Learning for the Full CTL Logic

In this section, we learn a DTMC $\hat{A}_W$ such that $\hat{A}_W$ and A have similar behaviors over all CTL formulas. This provides a much stronger result than on time-to-failure property, e.g., properties can involve liveness and fairness, and more importantly they are not known before the learning. Notice that PCTL [2] cannot be used, since an infinitesimal error on one >0 probability can change the probability of a PCTL formula from 0 to 1. (State)-CTL is defined as follows:

Definition 3. *Let Prop be the set of state names. (State)-CTL is defined by the following grammar* $\varphi ::= \bot \mid \top \mid p \mid \neg\varphi \mid \varphi \wedge \varphi \mid \varphi \vee \varphi \mid \varphi \wedge \varphi \mid \mathbf{AX}\varphi \mid \mathbf{EX}\varphi \mid \mathbf{AF}\varphi \mid \mathbf{EF}\varphi \mid \mathbf{AF}\varphi \mid \mathbf{EG}\varphi \mid \mathbf{AG}\varphi \mid \mathbf{E}(\varphi\mathbf{U}\varphi) \mid \mathbf{A}(\varphi\mathbf{U}\varphi)$*, with* $p \in$ *Prop.* **E***(xists) and* **A***(ll) are quantifiers on paths, ne***X***t,* **G***lobally,* **F***inally and* **U***ntil are path-specific quantifiers. Notice that some operators are redundant. A minimal set of operators is* $\{\top, \vee, \neg, \mathbf{EG}, \mathbf{EU}, \mathbf{EX}\}$.

As we want to compute the probability of *paths* satisfying a CTL formula, we consider the set Ψ of *path-CTL* properties, that is formulas φ of the form $\varphi = \mathbf{X}\varphi_1$, $\varphi = \varphi_1\mathbf{U}\varphi_2$, $\varphi = \mathbf{F}\varphi_1$ or $\varphi = \mathbf{G}\varphi_1$, with φ_1, φ_2 (state)-CTL formulas. For instance, the property considered in the previous section is $(\neg s_0)\mathbf{U}s_F$.

In this section, for the sake of simplicity, the finite set W of traces is obtained by observing paths till a state is seen twice on the path. Then, the reset action is used and another trace is obtained from another path. That is, a trace ω from W is of the form $\omega = \rho \cdot s \cdot \rho' \cdot s$, with $\rho \cdot s \cdot \rho'$ a loop-free path.

As explained in example 1, some additional knowledge on the system is necessary. In this section, we assume that the support of transition probabilities is known, i.e., for any state i, we know the set of states j such that $a_{ij} \neq 0$. This assumption is needed both for Theorem 5 and to apply Laplace smoothing.

6.1 Learning DTMCs with Laplace Smoothing

Let $\alpha > 0$. For any state s, let k_s be the number of successors of s, that we know by hypothesis, and $T = \sum_{s \in S} k_s$ be the number of non-zero transitions. Let W be a set of traces, n_{ij}^W the number of transitions from state i to state j, and $n_i^W = \sum_j n_{ij}^W$. The *estimator for* W *with Laplace smoothing* α is the DTMC $\hat{A}_W^\alpha = (\hat{a}_{ij})_{1 \leq i,j \leq m}$ given for all i, j by:

$$\hat{a}_{ij} = \frac{n_{ij}^W + \alpha}{n_i^W + k_i\alpha} \text{ if } a_{ij} \neq 0 \quad \text{and} \quad \hat{a}_{ij} = 0 \text{ otherwise}$$

In comparison with the frequency estimator, the Laplace smoothing adds for each state s a term α to the numerator and k_s times α to the denominator. This preserves the fact that $\hat{A}_W^\alpha$ is a Markov chain, and it ensures that $\hat{a}_{ij} \neq 0$ iff $a_{ij} \neq 0$. In particular, compared with the frequency estimator, it avoids creating zeros in the probability tables.

6.2 Conditioning and Probability Bounds

Using Laplace smoothing slightly changes the probability of each transition by an additive offset η. We now explain how this small error η impacts the error on the probability of a CTL property.

Let A be a DTMC, and A_η be a DTMC such that $A_\eta(i,j) \neq 0$ iff $A(i,j) \neq 0$ for all states i, j, and such that $\sum_j |A_\eta(i,j) - A(i,j)| \leq \eta$ for all states i. For all states $s \in S$, let $R(s)$ be the set of states i such that there exists a path from i to s. Let $R_*(s) = R(s) \setminus \{s\}$. Since both DTMCs have the same support, R (and also R_*) is equal for A and A_η. Given m the number of states, the conditioning of A for $s \in S$ and $\ell \leq m$ is:

$$\mathrm{Cond}_s^\ell(A) = \min_{i \in R_*(s)} \mathbb{P}_i^A(\mathbf{F}_{\leq \ell} \neg R_*(s))$$

i.e., the minimal probability from state $i \in R_*(s)$ to move away from $R_*(s)$ in at most ℓ steps. Let ℓ_s be the minimal value such that $\mathrm{Cond}_s^{\ell_s}(A) > 0$. This minimal ℓ_s exists as $\mathrm{Cond}_s^m(A) > 0$ since, for all $s \in S$ and $i \in R_*(s)$, there is at least one path reaching s from i (this path leaves $R_*(s)$), and taking a cycle-free path, we obtain a path of length at most m. Thus, the probability $\mathbb{P}_i^A(\mathbf{F}_{\leq m} \neg R_*(s))$ is at least the positive probability of the cylinder defined by this finite path. Formally,

Theorem 4. *Denoting φ the property of reaching state s in DTMC A, we have:*

$$|\gamma(A,\varphi) - \gamma(A_\eta,\varphi)| < \frac{\ell_s \cdot \eta}{Cond_s^{\ell_s}(A)}$$

Proof. Let v_s be the stochastic vector with $v_s(s) = 1$. We denote $v_0 = v_{s_0}$. Let $s \in S$. We assume that $s_0 \in R_*(s)$ (else $\gamma(A,\varphi) = \gamma(A_\eta,\varphi)$ and the result is trivial). Without loss of generality, we can also assume that $A(s,s) = A_\eta(s,s) = 1$ (as we are interested in reaching s at any step). With this assumption:

$$|\gamma(A,\varphi) - \gamma(A_\eta,\varphi)| = \lim_{t \to \infty} |v_0 \cdot (A^t - A_\eta^t) \cdot v_s|$$

We bound this error, through bounding by induction on t:

$$E(t) = \max_{i \in R_*(s)} |v_i \cdot (A^t - A_\eta^t) \cdot v_s|$$

We then have trivially:

$$|\gamma(A,\varphi) - \gamma(A_\eta,\varphi)| \leq \lim_{t \to \infty} E(t)$$

Note that for $i = s$, $\lim_{t\to\infty} v_i \cdot (A^t) \cdot v_s = 1 = \lim_{t\to\infty} v_i \cdot A_\eta^t \cdot v_s$, and thus their difference is null.

Let $t \in \mathbb{N}$. We let $j \in R_*(s)$ such that $E(t) = |v_j \cdot (A^t - A_\eta^t) \cdot v_s|$.

By the triangular inequality, introducing the term $v_j \cdot A^{\ell_s} A_\eta^{t-k} \cdot v_s - v_j \cdot A^{\ell_s} A_\eta^{t-k} \cdot v_s = 0$, we have:

$$E(t) \leq |v_j \cdot (A_\eta^t - A^{\ell_s} A_\eta^{t-\ell_s}) \cdot v_s| + |(v_j \cdot A^{\ell_s}) \cdot (A_\eta^{t-\ell_s} - A^{t-\ell_s}) \cdot v_s|$$

We separate vector $(v_j \cdot A^{\ell_s}) = w_1 + w_2 + w_3$ in three sub-stochastic vectors w_1, w_2, w_3: vector w_1 is over $\{s\}$, and thus we have $w_1 \cdot A_\eta^{t-\ell_s} = w_1 = w_1 \cdot A^{t-\ell_s}$, and the term cancels out. Vector w_2 is over states of $R_*(s)$, with $\sum_{i \in R_*} w_2[i] \leq (1 - \mathrm{Cond}_s^{\ell_s}(A))$, and we obtain an inductive term $\leq (1 - \mathrm{Cond}_s^{\ell_s}(A))E(t - \ell_s)$. Last, vector w_3 is over states not in $R(s)$, and we have $w_3 \cdot A_\eta^{t-\ell_s} \cdot v_s = 0 = w_3 \cdot A^{t-\ell_s} \cdot v_s$, and the term cancels out.

We also obtain that $|v_j \cdot (A_\eta^t - A^{\ell_s} A_\eta^{t-\ell_s}) \cdot v_s| \leq \ell_s \cdot \eta$. Thus, we have the inductive formula $E(t) \leq (1 - \mathrm{Cond}_s^{\ell_s}(A))E(t - \ell_s) + \ell_s \cdot \eta$. It yields for all $t \in \mathbb{N}$:

$$E(t) \leq (\ell_s \cdot \eta) \sum_{i=1}^{\infty} (1 - \mathrm{Cond}_s^{\ell_s}(A))^i$$

$$E(t) \leq \frac{\ell_s \cdot \eta}{Cond_s^{\ell_s}(A)} \qquad \square$$

We can extend this result from reachability to formulas of the form $S_0 \mathbf{U} S_F$, where S_0, S_F are subsets of states. This formula means that we reach the set of states S_F through only states in S_0 on the way.

We define $R(S_0, S_F)$ to be the set of states which can reach S_F using only states of S_0, and $R_*(S_0, S_F) = R(S_0, S_F) \setminus S_F$. For $\ell \in \mathbb{N}$, we let:

$$\mathrm{Cond}_{S_0, S_F}^{\ell}(A) = \min_{i \in R_*(S_0, S_F)} \mathbb{P}_i^A(\mathbf{F}_{\leq \ell} \neg R_*(S_0, S_F) \vee \neg S_0).$$

Now, one can remark that $\mathrm{Cond}_{S_0, S_F}(A) \geq \mathrm{Cond}_{S, S_F}(A) > 0$. Let $\mathrm{Cond}_{S_F}^{\ell}(A) = \mathrm{Cond}_{S, S_F}^{\ell}(A)$. We have $\mathrm{Cond}_{S_0, S_F}^{\ell}(A) \geq \mathrm{Cond}_{S_F}^{\ell}(A)$. As before, we let $\ell_{S_F} \leq m$ be the minimal ℓ such that $\mathrm{Cond}_{S_F}^{\ell}(A) > 0$, and obtain:

Theorem 5. *Denoting φ the property $S_0 \mathbf{U} S_F$, we have, given DTMC A:*

$$|\gamma(A, \varphi) - \gamma(A_\eta, \varphi)| < \frac{\ell_{S_F} \cdot \eta}{Cond_{S_F}^{\ell_{S_F}}(A)}$$

We can actually improve this conditioning: we defined it as the probability to reach S_F or $S \setminus R(S, S_F)$. At the price of a more technical proof, we can obtain a better bound by replacing S_F by the set of states $R_1(S_F)$ that have probability 1 to reach S_F. We let $\overline{R_*}(S_F) = R(S, S_F) \setminus R_1(S_F)$ the set of states that can reach S_F with < 1 probability, and define the *refined conditioning* as follows:

$$\overline{\mathrm{Cond}}_{S_F}^{\ell}(A) = \min_{i \in \overline{R_*}(S_F)} \mathbb{P}_i^A(\mathbf{F}_{\leq \ell} \neg \overline{R_*}(S_F))$$

6.3 Optimality of the Conditioning

We show now that the bound we provide in Theorem 4 is close to optimal.

Consider again DTMCs $A, \hat{A}$ in Fig. 3 from example 1, and formula $\mathbf{F}\, s_2$ stating that s_2 is eventually reached. The probabilities to satisfy this formula in $A, \hat{A}$ are respectively $\mathbb{P}^A(\mathbf{F}\, s_2) = \frac{1}{2}$ and $\mathbb{P}^{\hat{A}}(\mathbf{F}\, s_2) = \frac{1}{2} - \frac{\eta}{4\tau}$. Assume that A is the real system and that $\hat{A}$ is the DTMC we learned from A.

As we do not know precisely the transition probabilities in A, we can only compute the conditioning on $\hat{A}$ and not on A (it suffices to swap A and A_η in Theorem 4 and 5 to have the same formula using $\mathrm{Cond}(A_\eta) = \mathrm{Cond}(\hat{A})$). We have $R(s_2) = \{s_1, s_2\}$ and $R_*(s_2) = \overline{R_*}(s_2) = \{s_1\}$. The probability to stay in $R_*(s_2)$ after $\ell_{s_2} = 1$ step is $(1 - 2\tau)$, and thus $\mathrm{Cond}^1_{\{s_2\}}(\hat{A}) = \overline{\mathrm{Cond}}^1_{\{s_2\}}(\hat{A}) = 1-(1-2\tau) = 2\tau$. Taking $A_\eta = \hat{A}$, Theorem 5 tells us that $|\mathbb{P}^A(\mathbf{F}\, s_2) - \mathbb{P}^{\hat{A}}(\mathbf{F}\, s_2)| \leq \frac{\eta}{2\tau}$. Notice that on that example, using $\ell_{s_2} = m = 3$, we obtain $\mathrm{Cond}^3_{\{s_2\}}(\hat{A}) = 1 - (1 - 2\tau)^3 \approx 6\tau$, and we find a similar bound $\approx \frac{3\eta}{6\tau} = \frac{\eta}{2\tau}$.

Compare our bound with the exact difference $|\mathbb{P}^A(\mathbf{F}\, s_2) - \mathbb{P}^{\hat{A}}(\mathbf{F}\, s_2)| = \frac{1}{2} - (\frac{1}{2} - \frac{\eta}{4\tau}) = \frac{\eta}{4\tau}$. Our upper bound only has an overhead factor of 2, even while the conditioning is particularly bad (small) in this example.

6.4 PAC Bounds for $\sum_j |\hat{\boldsymbol{A}}_{\boldsymbol{W}}(\boldsymbol{i}, \boldsymbol{j}) - \boldsymbol{A}(\boldsymbol{i}, \boldsymbol{j})| \leq \boldsymbol{\eta}$

We use Theorem 1 in order to obtain PAC bounds. We use it to estimate individual transition probabilities, rather than the probability of a property.

Let W be a set of traces drawn with respect to A such that every $\omega \in W$ is of the form $\omega = \rho \cdot s \cdot \rho' \cdot s$. Recall for each state i, j of S, n_i^W is the number of transitions originating from i in W and n_{ij}^W is the number of transitions ss' in W. Let $\delta' = \frac{\delta}{m_{\text{stoch}}}$, where m_{stoch} is the number of *stochastic* states, i.e., with at least two outgoing transitions.

We want to sample traces until the empirical transition probabilities $\frac{n_{ij}^W}{n_i^W}$ are relatively close to the exact transition probabilities a_{ij}, for all $i, j \in S$. For that, we need to determine a stopping criteria over the number of state occurrences $(n_i)_{1 \leq i \leq m}$ such that:

$$\mathbb{P}\left(\exists i \in S, \sum_j \left| a_{ij} - \frac{n_{ij}^W}{n_i^W} \right| > \varepsilon\right) \leq \delta$$

First, note that for any observed state $i \in S$, if $a_{ij} = 0$ (or $a_{ij} = 1$), then with probability 1, $\frac{n_{ij}^W}{n_i^W} = 0$ (respectively $\frac{n_{ij}^W}{n_i^W} = 1$). Thus, for all $\varepsilon > 0$, $|a_{ij} - \frac{n_{ij}^W}{n_i^W}| < \varepsilon$ with probability 1. Second, for two distinct states i and i', the transition probabilities $\frac{n_{ij}^W}{n_i^W}$ and $\frac{n_{i'j'}^W}{n_{i'}^W}$ are independent for all j, j'.

Let $i \in S$ be a stochastic state. If we observe n_i^W transitions from i such that $n_i^W \geq \frac{2}{\varepsilon^2} \log\left(\frac{2}{\delta'}\right) \left[\frac{1}{4} - \left(\max_j |\frac{1}{2} - \frac{n_{ij}^W}{n_i^W}| - \frac{2}{3}\varepsilon\right)^2\right]$, then, according to Theorem 1,

$\mathbb{P}\left(\bigvee_{j=1}^{m} |a_{ij} - \frac{n_{ij}^W}{n_i^W}| > \varepsilon\right) \leq \delta'$. In particular, $\mathbb{P}\left(\max_{j\in S} |a_{ij} - \frac{n_{ij}^W}{n_i^W}| > \varepsilon\right) \leq \delta'$. Moreover, we have:

$$\begin{aligned}\mathbb{P}\left(\bigvee_{j=1}^{m} \max_{j\in S} |a_{ij} - \frac{n_{ij}^W}{n_i^W}| > \varepsilon\right) &\leq \sum_{j=1}^{m} \mathbb{P}\left(\max_{j\in S} |a_{ij} - \frac{n_{ij}^W}{n_i^W}| > \varepsilon\right) \\ &\leq m_{\text{stoch}}\delta' \\ &\leq \delta\end{aligned}$$

In other words, the probability that "there exists a state $i \in S$ such that the deviation between the exact and empirical outgoing transitions from i exceeds ε" is bounded by δ as soon as for each state $i \in S$, n_i^W satisfies the stopping rule of the algorithm of Chen using ε and the corresponding δ'. This gives the hypothesis $\sum_j |A_\eta(i,j) - A(i,j)| \leq \epsilon$ for all states i of Sect. 6.2.

6.5 A Matrix $\hat{A}_W$ Accurate for all CTL properties

We now use Laplace smoothing in order to ensure the other hypothesis $A_\eta(i,j) \neq 0$ iff $A(i,j) \neq 0$ for all states i, j. For all $i \in S$, we define the Laplace offset depending on the state i as $\alpha_i = \frac{(n_i^W)^2\varepsilon}{10\cdot k_i^2 \max_j n_{ij}^W}$, where k_i is the number of transitions from state i. This ensures that the error from Laplace smoothing is at most one tenth of the statistical error. Let $\alpha = (\alpha_i)_{1\leq i\leq m}$. From the sample set W, we output the matrix $\hat{A}_W^\alpha = (\hat{a}_{ij})_{1\leq i,j\leq m}$ with Laplace smoothing α_i for state i, i.e.:

$$\hat{a}_{ij} = \frac{n_{ij}^W + \alpha_i}{n_i^W + k_i\alpha_i} \text{ if } a_{ij} \neq 0 \quad \text{and} \quad \hat{a}_{ij} = 0 \text{ otherwise}$$

It is easy to check that we have for all $i, j \in S$: $\left|\hat{a}_{ij} - \frac{n_{ij}^W}{n_i^W}\right| \leq \frac{\varepsilon}{10\cdot k_i}$

That is, for all states i, $\sum_j \left|\hat{a}_{ij} - \frac{n_{ij}^W}{n_i^W}\right| \leq \frac{\varepsilon}{10}$. Using the triangular inequality:

$$\mathbb{P}\left(\exists i \in S, \sum_j |a_{ij} - \hat{a}_{ij}| > \frac{11}{10}\varepsilon\right) \leq \delta$$

For all $i \in S$, let $H^*(n_i^W, \epsilon, \delta') = \max_{j\in S} H(n_i^W, n_{ij}^W, \epsilon, \delta')$ be the maximal Chen bound over all the transitions from state i. Let $B(\hat{A}_W^\alpha) = \max_{S_F} \frac{\ell_{S_F}}{\text{Cond}_{S_F}^{\ell_{S_F}}(\hat{A}_W^\alpha)}$. Since in Theorem 5, the original model and the learned one have symmetric roles, by applying this theorem on $\hat{A}_W^\alpha$, we obtain that:

Theorem 6. *Given a set W of traces, for $0 < \epsilon < 1$ and $0 < \delta < 1$, if for all $i \in S$, $n_i^W \geq \left(\frac{11}{10} B(\hat{A}_W^\alpha)\right)^2 H^*(n_i^W, \epsilon, \delta')$, we have for any CTL property φ:*

$$\mathbb{P}(|\gamma(A, \varphi) - \gamma(\hat{A}_W^\alpha, \varphi)|) > \varepsilon) \leq \delta \tag{9}$$

Proof. First, $\hat{a}_{ij} \neq 0$ iff $a_{ij} \neq 0$, by definition of $\hat{A}_W^\alpha$. Second, $\mathbb{P}(\exists i, \sum_j |a_{ij} - \hat{a}_{ij}| > \frac{11}{10}\varepsilon) \leq \delta$. We can thus apply Theorem 5 on $\hat{A}_W^\alpha, A$ and obtain (9) for φ any formula of the form $S_1 \mathbf{U} S_2$. It remains to show that for any formula $\varphi \in \Psi$, we can define $S_1, S_2 \subseteq S$ such that φ can be expressed as $S_1 \mathbf{U} S_2$.

Consider the different cases: If φ is of the form $\varphi = \varphi_1 \mathbf{U} \varphi_2$ (it subsumes the case $\varphi = \mathbf{F}\varphi_1 = \top \mathbf{U} \varphi_1$) with φ_1, φ_2 CTL formulas, we define S_1, S_2 as the sets of states satisfying φ_1 and φ_2, and we have the equivalence (see [2] for more details). If $\varphi = X\varphi_2$, define $S_1 = \emptyset$ and S_2 as the set of states satisfying φ_2.

The last case is $\varphi = \mathbf{G}\varphi_1$, with φ_1 a CTL formula. Again, we define S_1 the set of states satisfying φ_1, and S_2 the set of states satisfying the CTL formula $\mathbf{AG}\varphi_1$. The probability of the set of paths satisfying $\varphi = \mathbf{G}\varphi_1$ is exactly the same as the probability of the set of paths satisfying $S_1 \mathbf{U} S_2$. □

6.6 Algorithm

We give more details about the learning process of a Markov Chain, accurate for every CTL formula. For completeness, we also provide in the extended version a similar algorithm for a time-to-failure property.

A path ω is observed from s_0 till a state is observed twice. Then ω is added to W and the reset operation is performed. We use Laplace smoothing to compute

Algorithm 1: Learning a matrix accurate for CTL

Data:
$\mathcal{S}, s_0, \delta, \varepsilon$

$W := \emptyset$
$m = |S|$
for all $s \in S$, $n_s^W := 0$
Compute $\hat{A} := \hat{A}_W^\alpha$
Compute $B := B(\hat{A})$
while $\exists s \in S, n_s^W < \left(\frac{11}{10} B(\hat{A})\right)^2 H^*(n_s^W, \epsilon, \frac{\delta}{m})$ **do**
    Generate a new trace $\omega := s_0\, \rho\, s_1\, \rho'\, s_1$, and reset $\mathcal{S}$
    for all $s \in S$, $n_s^W := n_s^W + n_s^{\{\omega\}}$
    add ω to W
    Compute $\hat{A} := \hat{A}_W^\alpha$
    Compute $B := B(\hat{A})$

Output: $\hat{A}_W^\alpha$

the corresponding matrix $\hat{A}^{\alpha}_{W}$. The error bound is computed on W, and a new path ω' is then being generated if the error bound is not as small as desired.

This algorithm is guaranteed to terminate since, as traces are generated, with probability 1, n_s^W tends towards ∞, $\hat{A}^{\alpha}_{W}$ tends towards A, and $B(\hat{A}^{\alpha}_{W})$ tends towards $B(A)$.

7 Evaluation and Discussion

In this section, we first evaluate Algorithm 1 on 5 systems which are crafted to evaluate the algorithm under different conditions (e.g., rare states). The objective of the evaluation is to provide some idea on how many samples would be sufficient for learning accurate DTMC estimations, and compare learning for all properties of CTL and learning for one time-to-failure property.

Then, we evaluate our algorithm on very large PRISM systems (millions or billions of states). Because of the number of states, we cannot learn a DTMC accurate for all properties of CTL there: it would ask to visit every single state a number of times. However, we can learn a DTMC for one specific (unbounded) property. We compare with an hypothesis testing algorithm from [31] which can handle the same unbounded property through a reachability analysis using the topology of the system.

Table 1. Average number of observed events N (and relative standard deviation in parenthesis) given $\varepsilon = 0.1$ and $\delta = 0.05$ for a time-to-failure property and for the full CTL logic using the refined conditioning $\overline{\text{Cond}}$.

	System 1	System 2	System 3	System 4	System 5
# states	3	3	30	64	200
# transitions	4	7	900	204	40,000
# events for time-to-failure	191 (16%)	991 (10%)	2,753 (7.4%)	1,386 (17.9%)	18,335 (7.2%)
# events for full CTL	1,463 (12.9%)	4,159 (11.7%)	8,404 (3.8%)	1,872,863	79,823 (1.7%)

7.1 Evaluation on Crafted Models

We first describe the 5 systems: Systems 1 and 2 are three-state models described in Fig. 1 and Fig. 2. Systems 3 (resp. 5) is a 30-state (resp. 200-states) clique in which every individual transition probability is 1/30 (resp. 1/200). System 4 is a 64-state system modeling failure and repair of 3 types of components (3 components each, 9 components in total), see the extended version for a full description of the system, including a PRISM [20] model for the readers interested to investigate this system in details.

We tested time-to-failure properties by choosing as failure states s_3 for Systems 1, 2, 3, 5, and the state where all 9 components fail for System 4.

We also tested Algorithm 1 (for full CTL logic) using the refined conditioning $\overline{\text{Cond}}$. We performed our algorithms 100 times for each model, except for full CTL on System 4, for which we only tested once since it is very time-consuming. We report our results in Table 1 for $\varepsilon = 0.1$ and $\delta = 0.05$. In particular, we output for each model its number of states and transitions. For each (set of) property, we provide the average number of observations (i.e. the number of samples times their average length) and the relative standard deviation (in parenthesis, that is the standard deviation divided by the average number of observed events).

The results show that we can learn a DTMC with more than 40000 stochastic transitions, such that the DTMC is accurate for all CTL formulas. Notice that for some particular systems such as System 4, it can take a lot of events to be observed before Algorithm 1 terminates. The reason is the presence of rare states, such as the state where all 9 components fail, which are observed with an extremely small probability. In order to evaluate the probabilities of CTL properties of the form: "if all 9 components fail, then CTL property φ is satisfied", this state needs to be explored many times, explaining the high number of events observed before the algorithm terminates. On the other hand, for properties that do not involve the 9 components failing as prior, such as time-to-failure, one does not need to observe this state even once to conclude that it has an extremely small probability to happen. This suggests that efficient algorithms could be developed for subsets of CTL formulas, e.g., in defining a subset of important events to consider. We believe that Theorem 4 and 5 could be extended to handle such cases. Over different runs, the results stay similar (notice the rather small relative standard deviation).

Comparing results for time-to-failure (or equivalently SMC) and for the full CTL logic is interesting. Excluding System 4 which involves rare states, the number of events that needs to be observed for the full CTL logic is 4.3 to 7 times more. Surprisingly, the highest difference is obtained on the smallest System 1. It is because every run of System 1 generated for time-to-failure is short ($s_1 s_2 s_1$ and $s_1 s_2 s_3$). However, in Systems 2,3 and 5, samples for time-to-failure can be much longer, and the performances for time-to-failure (or equivalently SMC) is not so much better than for learning a DTMC accurate for all CTL properties.

For the systems we tested, the unoptimized Cond was particularly large (more than 20) because for many states s, there was probability 0 to leave $R(s)$, and hence $\ell(s)$ was quite large. These are the cases where $\overline{\text{Cond}}$ is much more efficient, as then we can choose $\ell_s = 1$ as the probability to reach s from states in $R(s)$ is 1 ($R_1(s) = R(s)$ and $\overline{R_*(s)} = \emptyset$). We used $\overline{\text{Cond}}$ in our algorithm.

Finally, we evaluate experimental confidence by comparing the time-to-failure probabilities in the learned DTMC and the original system. We repeat our algorithms 1000 times on System 1 and 2 (with $\varepsilon = 0.1$ and $\delta = 0.05$). These probabilities differ by less than ε, respectively 999 and 995 times out of 1000. Specification (2) is thus largely fulfilled (the specification should be ensured 950 out of 1000 times), that empirically endorses our approach. Hence, while our PAC bound over-approximates the confidence in the learned system (which is unavoidable), it is not that far from experimental values.

7.2 Evaluation on Large Models

We also evaluated our algorithm on large PRISM models, ranging from hundreds of thousands to billions of states. With these numbers of states, we cannot use the more ambitious learning over all the properties of CTL, which would need to visit every states a number of times. However, we can use our algorithm for learning a DTMC which is accurate given a particular (unbounded) property: it will visit only a fraction of the states, which is enough to give a model accurate for that property, with a well-learned kernel of states and some other states representatives for the remaining of the runs. We consider three test-cases from PRISM, satisfying the property that the sample stops with a conclusion (yes or no) with probability 1. Namely, *herman, leader* and *egl*.

Table 2. Results for $\varepsilon = 0.01$ and $\delta = 0.001$ of our algorithm compared with sampling with reachability analysis [31], as reported in [14], page 20. Numbers of samples needed by our method are given by the Massart bound (resp. by the Okamoto-Chernoff bound in parenthesis). TO and MO means time out (> 15 minutes on an Opteron 6134) and memory out (> 5GB) respectively.

Model name	Size	Our learning method		Sampling with reachability analysis [31]	
		Samples	Path length	Samples	Path length
herman(17)	129M	506 (38K)	27	219	30
herman(19)	1162M	506 (38K)	40	219	38
herman(21)	10G	506 (38K)	43	219	48
leader(6, 6)	280K	506 (38K)	7.4	219	7
leader(6, 8)	>280K	506 (38K)	7.4	(MO)	(MO)
leader(6, 11)	>280K	506 (38K)	7.3	(MO)	(MO)
egl(15, 10)	616G	38K (38K)	470	1100	201
egl(20, 15)	1279T	38K (38K)	930	999	347
egl(20, 20)	1719T	38K (38K)	1200	(TO)	(TO)

Our prototype tool used in the previous subsection is implemented in Scilab: it cannot simulate very large systems of PRISM. Instead, we use PRISM to generate the samples needed for the learning. Hence, we report the usual Okamoto-Chernoff bound on the number of samples, which is what is implemented in PRISM. We also compare with the Massart bound used by the Chen algorithm (see Sect. 2.2), which is implemented in our tool and is more efficient as it takes into account the probability of the property.

For each model, we report its parameters, its *size*, i.e. its number of states, the number of *samples* needed using the Massart bound (the conservative Okamoto-Chernoff bound is in parenthesis), and the average *path length*. For comparison, we consider an hypothesis testing algorithm from [31] which can also handle unbounded properties. It uses the knowledge of the topology to do reachability analysis to stop the sampling if the property cannot be reached anymore. Hypothesis testing is used to decide with high confidence whether a probability exceeds a threshold or not. This requires less samples than SMC algorithms

which estimate probabilities, but it is also less precise. We chose to compare with this algorithm because as in our work, it does not require knowledge on the probabilities, such as a lower bound on the transition probabilities needed by e.g. [14]. We do not report runtime as they cannot be compared (different platforms, different nature of result, etc.).

There are several conclusions we can draw from the experimental results (shown in Table 2). First, the number of samples from our algorithm (Chen algorithm implementing the Massart bound) are larger than in the algorithm from [31]. This is because they do hypothesis testing, which requires less samples than even estimating the probability of a property, while we learn a DTMC accurate for this property. For *herman* and *leader*, the difference is small (2.5x), because it is a case where the Massart bound is very efficient (80 times better than Okamoto-Chernoff implemented in PRISM). The *egl* system is the worst-case for the Massart bound (the probability of the property is $\frac{1}{2}$), and it coincides with Okamoto-Chernoff. The difference with [31] is 40x in that case. Also, as shown in *egl*, paths in our algorithm can be a bit larger than in the algorithm from [31], where they can be stopped early by the reachability analysis. However, the differences are never larger than 3x. On the other hand, we learn a model representative of the original system for a given property, while [31] only provide a yes/no answer to hypothesis testing (performing SMC evaluating the probability of a property with the Massart bound would give exactly the same number of samples as we report for our learning algorithm). Last, the reachability analysis from [31] does time out or memory out on some complex systems, which is not the case with our algorithm.

8 Conclusion

In this paper, we provided theoretical grounds for obtaining global PAC bounds when learning a DTMC: we bound the error made between the behaviors of the model and of the system, formalized using temporal logics. While it is not possible to obtain a learning framework for LTL properties, we provide it for the whole CTL logic. For subsets of CTL, e.g. for a fixed timed-to-failure property, we obtain better bounds, as efficient as Statistical MC. Overall, this work should help in the recent trends of establishing trusted machine learning [16].

Our techniques are useful for designers of systems for which probabilities are governed by uncertain forces (e.g. error rates): in this case, it is not easy to have a lower bound on the minimal transition probability, but we can assume that the set of transitions is known. Technically, our techniques provides rationale to set the constant in Laplace smoothing, otherwise left to an expert to set.

Some cases remain problematic, such as systems where states are visited very rarely. Nevertheless, we foresee potential solutions involving rare event simulation [21]. This goes beyond the scope of this work and it is left to future work.

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Unbounded-Time Safety Verification of Stochastic Differential Dynamics

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Abstract. In this paper, we propose a method for bounding the probability that a stochastic differential equation (SDE) system violates a safety specification over the infinite time horizon. SDEs are mathematical models of stochastic processes that capture how states evolve continuously in time. They are widely used in numerous applications such as engineered systems (e.g., modeling how pedestrians move in an intersection), computational finance (e.g., modeling stock option prices), and ecological processes (e.g., population change over time). Previously the safety verification problem has been tackled over finite and infinite time horizons using a diverse set of approaches. The approach in this paper attempts to connect the two views by first identifying a finite time bound, beyond which the probability of a safety violation can be bounded by a negligibly small number. This is achieved by discovering an exponential barrier certificate that proves exponentially converging bounds on the probability of safety violations over time. Once the finite time interval is found, a finite-time verification approach is used to bound the probability of violation over this interval. We demonstrate our approach over a collection of interesting examples from the literature, wherein our approach can be used to find tight bounds on the violation probability of safety properties over the infinite time horizon.

Keywords: Stochastic differential equations (SDEs) · Unbounded safety verification · Failure probability bound · Barrier certificates

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1 Introduction

In this paper, we investigate the problem of verifying probabilistic safety properties for continuous stochastic dynamics modeled by stochastic differential equations (SDEs). The study of SDEs dates back to the 1900s when, e.g., Einstein used SDEs to model the phenomenon of Brownian motion [10]. Since then, SDEs have witnessed numerous applications including models of disturbances in engineered systems ranging from wind forces [37] to pedestrian motion [14]; models of financial instruments such as options [5]; and models of biological/ecological processes for instance predator-prey models [25]. In the meantime, SDEs are hard to reason about: they are defined using ideas from stochastic calculus that reimagine basic concepts such as integration in order to conform to the basic laws of probability and stochastic processes [24].

There are many important verification problems for SDEs. Prominent topics include the safety verification problem which seeks to know the probability that a given SDE with specified initial conditions will enter an unsafe region (or leave a safe region) over a given time horizon. Generally, safety verification can be performed over a finite-time horizon setting, wherein the probability is sought over a finite time interval $[0, T]$. On the other hand, the infinite-time horizon problem seeks a bound on the probability of satisfying a safety property over the unbounded time horizon $[0, \infty)$. A handful of methods have been proposed for verifying SDE systems, such as the barrier certificate-based methods over both the infinite time horizon [27] and finite time horizons [35], the moment optimization-based method over finite time horizons [33] and the Hamilton-Jacobi-based method over the infinite time horizon [16]. The novelty of our work lies in the reduction of infinite-time horizon verification problems to finite time problems.

In this paper, we propose a novel reduction-based method to verify unbounded-time safety properties of stochastic systems modeled as nonlinear polynomial SDEs. We employ a similar idea as in [11] (for verifying delay differential equations) that reduces the safety verification problem over the infinite time horizon to the one over a finite time interval. This is achieved by computing an *exponential stochastic barrier certificate* which witnesses an exponentially decreasing upper bound on the probability that a target system violates a given safety specification. Consequently, for any $\epsilon > 0$, we can identify a time instant T beyond which the violation (a.k.a. failure) probability is smaller than the negligibly small cutoff ϵ. The reduced bounded-time safety verification problem over $[0, T]$ can hence be tackled by any of the available methods. We furthermore present an alternative method to address the reduced finite-time horizon verification problem based on the discovery of a *time-dependent stochastic barrier certificate*. We show that both the exponential and the time-dependent stochastic barrier certificate can be synthesized by respectively solving a pertinent *semidefinite programming* (SDP) [38] optimization problem. Experimental results on some interesting examples taken from the literature demonstrated the effectiveness of the reduction and that our method often produces tighter bounds on the failure probability. Our approach has some broad similarities to related approaches in symbolic execution of probabilistic programs that conclude facts

about infinitely many behaviors by analyzing finitely many paths in the program that account for a sufficient probability among all the behaviors [31].

Contributions. The main contributions of this work can be summarized as follows: (1) We reduce the unbounded-time safety verification of stochastic systems to a bounded one, based on an exponentially decreasing bound on the failure probability which guarantees the dominance of the overall failure probability by the truncated finite time horizon. (2) We show how the obtained bound on the overall failure probability is tighter than that produced by existing methods for some interesting SDEs.

Related Work. The use of mathematical models of processes–ranging from finite state machines to various types of differential equations–has allowed us to reason about rich behaviors of Cyber-Physical Systems produced by the interaction between digital computers and physical plants [29]. In this regard, many modeling formalisms have been studied including finite state machines, ordinary differential equations (ODEs), timed automata, hybrid automata, etc. [8], on top of which a large variety of verification problems have been extensively investigated, e.g., safety verification through reachability analysis and temporal logic verification [3].

In the existing literature on formal verification, ODEs are often used to describe the behavior of deterministic continuous-time systems. However, these models have been shown over-simplistic in many applications that involve time delays, nondeterministic inputs and stochastic noises. SDEs hence arose as an important class of models that have been employed in practical domains covering, among others [24], financial models such as the famous Black-Scholes model used extensively in the theory of options pricing [5], wind disturbances [37], human pedestrian motion [14] and ecological models [25].

In what follows, we place our work in the context of formal verification techniques tailored for stochastic differential dynamics modeled as SDEs, and discuss contributions thereof that are highly related to our approach. Unbounded-time stochastic safety verification of SDE systems was first studied by Prajna et al. in [27,28], where a typical supermartingale was employed as a stochastic barrier certificate followed by computational conditions derived from Doob's martingale inequality [15]. Thereafter, the stochastic barrier certificate-based method was extended to cater for bounded-time safety verification by Steinhardt and Tedrake [35] by leveraging a relaxed formulation called c-martingale for locally stable systems. The barrier certificate-based method by Prajna et al. (ibid.) for unbounded-time safety verification often leads to conservative bound on the failure probability. On the other hand, Steinhardt and Tedrake (ibid.) established impressive probability bounds but only for finite time horizons. In order to reduce the conservativeness, we propose a method of reducing the unbounded safety verification to a bounded one. Although our method in this paper is also based on the construction of stochastic barrier certificates, the gain of stochastic barrier certificates only helps to identify a finite time interval such that the violation probability of interest beyond this time interval is arbitrarily negligibly small. A time-dependent barrier certificate is further proposed to solve the resulting

bounded-time safety verification. The Unbounded-time safety verification problem has also been studied by Koutsoukos and Riley [16], who linked the reachability probability to the viscosity solution of certain Hamilton-Jacobi partial differential equations, under restrictions on bounded state space and non-degenerate diffusion. Grid-based numerical approaches, e.g., the finite difference method in [16] and the level set method in [22], are traditionally used to solve these equations, leading to the fact that the Hamilton-Jacobi reachability method only scales well to systems of special structures. More recently, a novel constraint solving-based method has been proposed in [20] for algebraically over- and under-approximating the reachability probability, which is nevertheless limited to bounded-time safety verification. In addition to the abovementioned methods, we refer the readers to [7] for a Dirichlet form-based method for stochastic hybrid systems featuring "nice" Markov properties, while to [6,18,39] and [1,17] respectively for related contributions in statistical and discrete/numerical methods for stochastic verification and control.

Finally, we mention a relation between the ideas in this paper and previously proposed ideas for (non-stochastic) ODEs due to Sogokon et al. [34]. The key similarity lies in the use of a non-negative matrix through which a vector of functions whose derivatives are related to their current value. Whereas Sogokon et al. explored this idea for ODEs, we do so for SDEs. Another significant difference, in our work, is that we use the super-martingale functions to identify a time horizon $[0, T]$ and bound the probability of safety violation beyond T.

The reminder of this paper is structured as follows. Section 2 introduces stochastic differential dynamics modeled by SDEs and the unbounded-time safety verification problem of interest. Section 3 elucidates the reduction of unbounded safety verification to bounded ones based on the witness of stochastic barrier certificates. Section 4 presents the SDP formulation for discovering such barrier certificates over the reduced bounded time interval. After demonstrating our method on several examples in Sect. 5, we conclude the paper in Sect. 6.

2 Problem Formulation

Notations. Let $\mathbb{R}$ be the set of real numbers. For a vector $x \in \mathbb{R}^n$, x_i refers to its i-th component and $|x|$ denotes the ℓ^2-norm. Particularly, $\mathbf{0}$ and $\mathbf{1}$ denote respectively the vector of zeros and ones of appropriate dimension, and the comparison between vectors, e.g., $x \leq \mathbf{0}$, is component-wise. We define for $\delta > 0$, $\mathfrak{B}(x, \delta) \mathrel{\widehat{=}} \{x' \in \mathbb{R}^n \mid |x' - x| \leq \delta\}$ as the δ-closed ball centered at x. We abuse the notation $|\cdot|$ for an $m \times n$ matrix M as $|M| \mathrel{\widehat{=}} \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} |M_{ij}|^2}$. The exponential of a square matrix $M \in \mathbb{R}^{n \times n}$, denoted by e^M, is the $n \times n$ matrix given by the power series $\mathrm{e}^M \mathrel{\widehat{=}} \sum_{k=0}^{\infty} \frac{1}{k!} M^k$. For a set $\mathcal{X} \subseteq \mathbb{R}^n$, $\partial\mathcal{X}$, $\overline{\mathcal{X}}$ and $\mathcal{X}^\circ$ denote respectively the boundary, the closure and the interior of $\mathcal{X}$. Let C^k be the space of functions on $\mathbb{R}$ with continuous derivatives up to order k; a function $f(t, x) \colon \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}$ is in $C^{1,2}(\mathbb{R} \times \mathbb{R}^n)$ if $f \in C^1$ w.r.t. $t \in R$ and $f \in C^2$ w.r.t. $x \in \mathbb{R}^n$.

Let $(\Omega, \mathcal{F}, P)$ be a probability space, where Ω is a sample space, $\mathcal{F} \subseteq 2^\Omega$ is a σ-algebra on Ω, and $P\colon \mathcal{F} \to [0,1]$ is a probability measure on the measurable space $(\Omega, \mathcal{F})$. A *random variable* X defined on the probability space $(\Omega, \mathcal{F}, P)$ is an $\mathcal{F}$-measurable function $X\colon \Omega \to \mathbb{R}^n$; its *expectation* (w.r.t. P) is denoted by $E[X]$. Every random variable X induces a probability measure $\mu_X\colon \mathcal{B} \to [0,1]$ on $\mathbb{R}^n$, defined as $\mu_X(B) \mathrel{\widehat{=}} P(X^{-1}(B))$ for Borel sets B in the Borel σ-algebra $\mathcal{B}$ on $\mathbb{R}^n$. μ_X is called the *distribution of* X; its *support set* is $\mathtt{supp}(\mu_X) \mathrel{\widehat{=}} \overline{\bigcup_{\mu_X(B)>0} B}$, which will also be referred to as the support of X.

A (continuous-time) *stochastic process* is a parametrized collection of random variables $\{X_t\}_{t\in T}$ where the parameter space T is interpreted as, unless explicitly notated in this paper, the halfline $[0,\infty)$. We sometimes further drop the brackets in $\{X_t\}$ when it is clear from the context. A collection $\{\mathcal{F}_t \mid t \geq 0\}$ of σ-algebras of sets in $\mathcal{F}$ is a *filtration* if $\mathcal{F}_t \subseteq \mathcal{F}_{t+s}$ for $t, s \in [0,\infty)$. Intuitively, $\mathcal{F}_t$ carries the information known to an observer at time t. A random variable $\tau\colon \Omega \to [0,\infty)$ is called a *stopping time* w.r.t. some filtration $\{\mathcal{F}_t \mid t \geq 0\}$ of $\mathcal{F}$ if $\{\tau \leq t\} \in \mathcal{F}_t$ for all $t \geq 0$. A stochastic process $\{X_t\}$ adapted to a filtration $\{\mathcal{F}_t \mid t \geq 0\}$ is called a *supermartingale* if $E[X_t] < \infty$ for any $t \geq 0$ and $E[X_t \mid \mathcal{F}_s] \leq X_s$ for all $0 \leq s \leq t$. That is, the conditional expected value of any future observation, given all the past observations, is no larger than the most recent observation.

Stochastic Differential Dynamics. We consider a class of dynamical systems featuring stochastic differential dynamics governed by time-homogeneous SDEs of the form[1]

$$\mathrm{d}X_t = b(X_t)\ \mathrm{d}t + \sigma(X_t)\ \mathrm{d}W_t, \quad t \geq 0 \tag{1}$$

where $\{X_t\}$ is an n-dimensional continuous-time stochastic process, $\{W_t\}$ denotes an m-dimensional Wiener process (standard Brownian motion), $b\colon \mathbb{R}^n \to \mathbb{R}^n$ is a vector-valued polynomial flow field (called the *drift coefficient*) modeling deterministic evolution of the system, and $\sigma\colon \mathbb{R}^n \to \mathbb{R}^{n\times m}$ is a matrix-valued polynomial flow field (called the *diffusion coefficient*) that encodes the coupling of the system to Gaussian white noise $\mathrm{d}W_t$.

Suppose there exists a Lipschitz constant D s.t. $|b(x) - b(y)| + |\sigma(x) - \sigma(y)| \leq D\,|x - y|$ holds for all $x, y \in \mathbb{R}^n$. Then, given an initial state (a random variable) X_0, an SDE of the form (1) has a unique *solution* which is a stochastic process $X_t(\omega) = X(t,\omega)\colon [0,\infty) \times \Omega \to \mathbb{R}^n$ satisfying the stochastic integral equation (à la Itô's interpretation)

$$X_t = X_0 + \int_0^t b(X_s)\ \mathrm{d}s + \int_0^t \sigma(X_s)\ \mathrm{d}W_s. \tag{2}$$

The solution $\{X_t\}$ in Eq. (2) is also referred to as an *(Itô) diffusion process*, and will be denoted by X_t^{0,X_0} (or simply $X_t^{X_0}$), if necessary, to indicate the initial condition X_0 at $t = 0$.

A great deal of information about a diffusion process can be encoded in a partial differential operator termed the *infinitesimal generator*, which generalizes

[1] The general time-inhomogeneous case with time-dependent b and σ can be reduced to this form (cf. [24, Chap. 10]).

the Lie derivative that captures the evolution of a function along the diffusion process:

Definition 1 (Infinitesimal generator [24]). *Let $\{X_t\}$ be a (time-homogeneous) diffusion process in $\mathbb{R}^n$. The* infinitesimal generator $\mathcal{A}$ of X_t *is defined by*

$$\mathcal{A}f(s,x) = \lim_{t \downarrow 0} \frac{E^{s,x}\left[f(s+t, X_t)\right] - f(s,x)}{t}, \quad x \in \mathbb{R}^n.$$

The set of functions $f\colon \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}$ s.t. the limit exists at (s,x) is denoted by $\mathcal{D}_{\mathcal{A}}(s,x)$, while $\mathcal{D}_{\mathcal{A}}$ denotes the set of functions for which the limit exists for all $(s,x) \in \mathbb{R} \times \mathbb{R}^n$.

In subsequent sections, the readers may find applications of the operator $\mathcal{A}$ to a vector-valued function in a component-wise manner. The relation between $\mathcal{A}$ and the coefficients b, σ in SDE (1) is captured by the following result:

Lemma 1 [24]. *Let $\{X_t\}$ be a diffusion process defined by Eq. (1). If $f \in C^{1,2}(\mathbb{R} \times \mathbb{R}^n)$ with compact support, then $f \in \mathcal{D}_{\mathcal{A}}$ and*

$$\mathcal{A}f(t,x) = \frac{\partial f}{\partial t} + \sum_{i=1}^{n} b_i(x) \frac{\partial f}{\partial x_i} + \frac{1}{2} \sum_{i,j} (\sigma\sigma^{\mathsf{T}})_{ij} \frac{\partial^2 f}{\partial x_i \partial x_j}.$$

As a stochastic generalization of the Newton-Leibniz axiom, Dynkin's formula gives the expected value of any adequately smooth function of an Itô diffusion at a stopping time:

Theorem 1 (Dynkin's formula [9]). *Let $\{X_t\}$ be a diffusion process in $\mathbb{R}^n$. Suppose τ is a stopping time with $E[\tau] < \infty$, and $f \in C^{1,2}(\mathbb{R} \times \mathbb{R}^n)$ with compact support. Then*

$$E^{h,x}\left[f(\tau, X_\tau)\right] = f(h,x) + E^{h,x}\left[\int_0^\tau \mathcal{A}f(s, X_s)\, \mathrm{d}s\right].$$

In order to specify the behavior of an Itô diffusion across the domain boundary, we introduce the concept of *stopped process*, which is a stochastic process that is forced to have the same value after a prescribed (possibly random) time.

Definition 2 (Stopped process [12]). *Given a stopping time τ and a stochastic process $\{X_t\}$, the* stopped process $\{X_t^\tau\}$ *is defined by*

$$X^\tau(t,\omega) \triangleq X_{t \wedge \tau}(\omega) = \begin{cases} X(t,\omega) & \text{if } t \le \tau(\omega), \\ X(\tau(\omega),\omega) & \text{otherwise.} \end{cases}$$

Remark 1. By definition, a stopped process preserves, among others, continuity and the Markov property, and hence the aforementioned results on a stochastic process apply also to a stopped process.

Now consider a stochastic system modeled by an SDE of the form (1) that evolves "within" a not necessarily bounded set $\mathcal{X} \subseteq \mathbb{R}^n$. Since the solution $\{X_t\}$ of Eq. (1) may escape from $\mathcal{X}$ at any time instant $t > 0$, due to the unbounded nature of Gaussian, we define a stopped process $\tilde{X}_t \widehat{=} X_{t \wedge \tau_{\mathcal{X}}}$ with $\tau_{\mathcal{X}} \widehat{=} \inf\{t \mid X_t \notin \mathcal{X}\}$. $\tilde{X}_t$ hence represents the process that will stop at the boundary of $\mathcal{X}$. Denote the infinitesimal generator of the stopped process as $\tilde{\mathcal{A}}$. One plausible property here is that, for all compactly-supported $f \in C^{1,2}(\mathbb{R} \times \mathbb{R}^n)$,

$$\tilde{\mathcal{A}} f(t,x) = \begin{cases} \mathcal{A} f(t,x) & \text{for } x \in \mathcal{X}^\circ, \\ \frac{\partial f}{\partial t}(t,x) & \text{for } x \in \partial\mathcal{X}. \end{cases} \tag{3}$$

The ∞-Safety Problem. Given an SDE of the form (1), a (not necessarily bounded[2]) domain set $\mathcal{X} \subseteq \mathbb{R}^n$, an initial set $\mathcal{X}_0 \subset \mathcal{X}$, and an unsafe set $\mathcal{X}_u \subset \mathcal{X}$. We aim to bound the failure probability

$$P\left(\exists t \in [0,\infty) \colon \tilde{X}_t \in \mathcal{X}_u\right),$$

for any initial state X_0 whose support lies within $\mathcal{X}_0$. Accordingly, the *T-safety problem*, with $T < \infty$, refers to the problem where one aims to bound the failure probability within the finite time horizon $[0, T]$.

Remark 2. Roughly speaking, if we denote by ϕ the proposition "$\tilde{X}_t$ evolves within $\mathcal{X}$" and by ψ the proposition "$\tilde{X}_t$ evolves into $\mathcal{X}_u$", then the above ∞-safety problem asks for a bound on the probability that the LTL formula $\phi \mathcal{U} \psi$ holds.

3 Reducing ∞-Safety to T-Safety

We dedicate this section to the reduction of the ∞-safety problem to its bounded counterpart. Observe that for any $0 \leq T < \infty$,

$$P(\exists t \geq 0 \colon \tilde{X}_t \in \mathcal{X}_u) \leq P(\exists t \in [0,T] \colon \tilde{X}_t \in \mathcal{X}_u) + P(\exists t \geq T \colon \tilde{X}_t \in \mathcal{X}_u).$$

The key idea behind our approach is to first compute an exponentially decreasing bound on the *tail failure probability* over $[T^*, \infty)$ (the computation of $T^* \geq 0$ will be shown later), and then for any constant $\epsilon > 0$, we can identify (out of the exponentially decreasing bound) a time instant $\tilde{T} \geq T^*$ such that $P(\exists t \geq \tilde{T} \colon \tilde{X}_t \in \mathcal{X}_u) \leq \epsilon$. The overall bound on the failure probability over $[0, \infty)$ can consequently be obtained by solving the truncated $\tilde{T}$-safety problem.

[2] In practice, if we can specify $\mathcal{X}$ based on prior knowledge when modeling a physical system, then the larger $\mathcal{X}$ we choose, the greater (bound on) failure probability we will obtain.

3.1 Exponentially Decreasing Bound on the Tail Failure Probability

We first state a result that gives conditions when a linear map keeps vector inequality:

Lemma 2 [4, Chap. 4]**.** *For a matrix $M \in \mathbb{R}^{n\times n}$,*

- $\forall x, y \in \mathbb{R}^n : x \le y \implies Mx \le My$ *iff* M *is* non-negative*, i.e., $M_{ij} \ge 0$ for all $1 \le i, j \le n$.*
- *The matrix e^{Mt} is non-negative for all $t \ge 0$ iff M is* essentially non-negative*, i.e., $M_{ij} \ge 0$ for $i \ne j$.*

The existence of an exponentially decreasing bound on the tail failure probability relies on a witness of a supermartingale of the exponential type:

Theorem 2. *Suppose there exists an essentially non-negative matrix $\Lambda \in \mathbb{R}^{m\times m}$, together with an m-dimensional polynomial function (termed* exponential stochastic barrier certificate*) $V(x) = (V_1(x), V_2(x), \ldots, V_m(x))^\mathsf{T}$, with $V_i \colon \mathbb{R}^n \to \mathbb{R}$ for $1 \le i \le m$, satisfying*[3,4]

$$V(x) \ge \mathbf{0} \quad \text{for } x \in \mathcal{X}, \tag{4}$$
$$\mathcal{A}V(x) \le -\Lambda V(x) \quad \text{for } x \in \mathcal{X}, \tag{5}$$
$$\Lambda V(x) \le \mathbf{0} \quad \text{for } x \in \partial\mathcal{X}. \tag{6}$$

Define a function

$$F(t, x) \mathrel{\widehat{=}} \mathrm{e}^{\Lambda t} V(x),$$

then every component of $F(t, \tilde{X}_t)$ is a supermartingale.

Proof. For cases with a bounded domain $\mathcal{X}$, one can trivially extend the domain of $F(t, x)$ s.t. F is compactly-supported, and thus Dynkin's formula in Theorem 1 applies immediately. For cases where $\mathcal{X}$ is unbounded, we introduce a stopping time

$$\tau_\delta \mathrel{\widehat{=}} \inf\left\{t \;\middle|\; F\left(t, \tilde{X}_t\right) \ge \mathfrak{B}(\mathbf{0}, \delta)\right\},$$

and denote by $X_t^{(\delta)} \mathrel{\widehat{=}} (t \wedge \tau_\delta, \tilde{X}_{t\wedge\tau_\delta})$ the corresponding stopped process involving the timeline, and by $\mathcal{A}^{(\delta)}$ the corresponding infinitesimal generator. Then $X_t^{(\delta)}$ evolves within the δ-closed ball $\mathfrak{B}(\mathbf{0}, \delta)$ and hence boils down to the case with a bounded domain. Moreover, by Eq. (3), we have

$$\begin{aligned}\mathcal{A}^{(\delta)} F\left(X_t^{(\delta)}\right) &= \mathcal{A}^{(\delta)} F\left(t \wedge \tau_\delta, \tilde{X}_{t\wedge\tau_\delta}\right) \\ &= \begin{cases} 0 \quad \text{if } \tau_\delta(\omega) \le t, \\ \frac{\partial F}{\partial t}(t, X_t) + \mathrm{e}^{\Lambda t}\mathcal{A}V(X_t) \le 0 \quad \text{if } \tau_\delta(\omega) > t \wedge \tau_{\mathcal{X}}(\omega) > t, \\ \frac{\partial F}{\partial t}(t, X_t) \le 0 \quad \text{if } \tau_\delta(\omega) > t \wedge \tau_{\mathcal{X}}(\omega) \le t, \end{cases}\end{aligned}$$

[3] Condition (5) is slightly stronger than the corresponding one used in [27,28], yet will lead to an exponentially decreasing bound on the tail failure probability in return.

[4] Condition (6) is to ensure that when $\tilde{X}_t$ stops at the boundary of $\mathcal{X}$, we still have $\tilde{\mathcal{A}}V(x) \le -\Lambda V(x)$ for $x \in \partial\mathcal{X}$. If $\mathcal{X} = \mathbb{R}^n$, however, this condition can be omitted.

where $\tau_{\mathcal{X}}$ represents the time instant when escaping from the state space $\mathcal{X}$. Note that the second and the third case hold due to the non-negativity of $\mathrm{e}^{\Lambda t}$ (as Λ is essentially non-negative), which implies that $\mathrm{e}^{\Lambda t}$ preserves vector inequalities (5) and (6). Hence by Dynkin's formula (in a component-wise manner), for fixed $t, h \in [0, \infty)$, we have

$$\begin{aligned} E\left[F\left((t+h)\wedge\tau_\delta, \tilde{X}_{(t+h)\wedge\tau_\delta}\right) \mid \mathcal{F}_h\right] &= E^{X_h^{(\delta)}}\left[F\left(X_{t+h}^{(\delta)}\right)\right] \\ &= F\left(X_h^{(\delta)}\right) + E^{X_h^{(\delta)}}\left[\int_0^t \mathcal{A}^{(\delta)} F\left(X_s^{(\delta)}\right) \mathrm{d}s\right] \\ &\leq F\left(X_h^{(\delta)}\right) \\ &= F\left(h\wedge\tau_\delta, \tilde{X}_{h\wedge\tau_\delta}\right). \end{aligned}$$

Since $F(t,x) > \mathbf{0}$, by Fatou's lemma, we have

$$\begin{aligned} E\left[F\left(t+h, \tilde{X}_{t+h}\right) \mid \mathcal{F}_h\right] &= E\left[\liminf_{\delta\to\infty} F\left((t+h)\wedge\tau_\delta, \tilde{X}_{(t+h)\wedge\tau_\delta}\right) \mid \mathcal{F}_h\right] \\ &\leq \liminf_{\delta\to\infty} E\left[F\left((t+h)\wedge\tau_\delta, \tilde{X}_{(t+h)\wedge\tau_\delta}\right) \mid \mathcal{F}_h\right] \\ &\leq \liminf_{\delta\to\infty} F\left(h\wedge\tau_\delta, \tilde{X}_{h\wedge\tau_\delta}\right) \\ &\leq F\left(h, \tilde{X}_h\right). \end{aligned}$$

It follows consequently that every component of $F(t, \tilde{X}_t)$ is a supermartingale. □

We will show in Sect. 4 that the synthesis of the exponential stochastic barrier certificate $V(x)$ (and thereby the function $F(t,x)$) boils down to solving a pertinent SDP optimization problem.

In order to further establish the relation between the exponential supermartingale $F(t, \tilde{X}_t)$ (and thereby $V(x)$) and the bound on tail failure probability, we recall Doob's maximal inequality for supermartingales, which gives a bound on the probability that a non-negative supermartingale exceeds some given value over a given time interval:

Lemma 3 (Doob's supermartingale inequality [15]). *Let $\{X_t\}_{t>0}$ be a right continuous non-negative supermartingale adapted to a filtration $\{\mathcal{F}_t \mid t > 0\}$. Then for any $\lambda > 0$,*

$$\lambda P\left(\sup_{t\geq 0} X_t \geq \lambda\right) \leq E[X_0].$$

The following theorem claims an intermediate fact that will later reveal the exponentially decreasing bound on the tail failure probability.

Theorem 3. *Suppose the conditions in Theorem 2 are satisfied. Then for any $T \geq 0$ and any positive vector $\gamma \in \mathbb{R}^m$,*

$$P\left(\sup_{t\geq T} V\left(\tilde{X}_t\right) \geq \sup_{t\geq T}\left(\mathrm{e}^{-\Lambda t}\gamma\right)\right) \leq E\left[V_i(X_0)\right]/\gamma_i \tag{7}$$

holds for all $i \in \{1, \ldots, m\}$.

Proof. Observe the following chain of (in-)equalities:

$$\begin{aligned}
P\left(\sup_{t\geq T} V\left(\tilde{X}_t\right) \geq \sup_{t\geq T}\left(\mathrm{e}^{-\Lambda t}\gamma\right)\right) &\leq P\left(\exists t \geq T\colon V\left(\tilde{X}_t\right) \geq \mathrm{e}^{-\Lambda t}\gamma\right) \\
&\leq P\left(\exists t \geq T\colon \mathrm{e}^{\Lambda t} V\left(\tilde{X}_t\right) \geq \gamma\right) && \text{[non-negative } \mathrm{e}^{\Lambda t}\text{]} \\
&= P\left(\sup_{t\geq T} F\left(t, \tilde{X}_t\right) \geq \gamma\right) \\
&\leq P\left(\sup_{t\geq T} F_i\left(t, \tilde{X}_t\right) \geq \gamma_i\right) \\
&\leq E\left[F_i\left(T, \tilde{X}_T\right)\right]/\gamma_i && \text{[Lemma 3]} \\
&\leq E\left[V_i\left(X_0\right)\right]/\gamma_i && \text{[Theorem 2]}
\end{aligned}$$

which holds for any $i \in \{1, 2, \cdots, m\}$. This completes the proof. □

Now, we are ready to give the exponentially decreasing bound on the tail failure probability derived from Theorem 3. We start by considering the simple case where the barrier certificate $V(x)$ is a scalar function, i.e., with $m = 1$.

Proposition 1. *Suppose there exists a positive constant* $\Lambda \in \mathbb{R}$ *and a scalar function* $V\colon \mathbb{R}^n \to \mathbb{R}$ *satisfying Theorem 2. Then,*

$$P\left(\sup_{t\geq T} V\left(\tilde{X}_t\right) \geq \gamma\right) \leq \frac{E\left[V(X_0)\right]}{\mathrm{e}^{\Lambda T}\gamma} \tag{8}$$

holds for any $\gamma > 0$ *and* $T \geq 0$. *Moreover, if there exists* $l > 0$ *such that*

$$V(x) \geq l \quad \text{for all } x \in \mathcal{X}_u,$$

then

$$P\left(\exists t \geq T\colon \tilde{X}_t \in \mathcal{X}_u\right) \leq \frac{E[V(X_0)]}{\mathrm{e}^{\Lambda T} l} \tag{9}$$

holds for any $T \geq 0$.

Proof. Equation (8) holds since

$$\begin{aligned}
P\left(\sup_{t\geq T} V\left(\tilde{X}_t\right) \geq \gamma\right) &= P\left(\sup_{t\geq T} V\left(\tilde{X}_t\right) \geq \mathrm{e}^{-\Lambda T}\left(\mathrm{e}^{\Lambda T}\gamma\right)\right) \\
&\leq P\left(\sup_{t\geq T} V\left(\tilde{X}_t\right) \geq \sup_{t\geq T}\left(\mathrm{e}^{-\Lambda t}\left(\mathrm{e}^{\Lambda T}\gamma\right)\right)\right) \\
& && \text{[monotonicity on } t\text{]} \\
&\leq \frac{E[V(X_0)]}{\mathrm{e}^{\Lambda T}\gamma}. && \text{[Theorem 3]}
\end{aligned}$$

For Eq. (9), it is immediately obvious that

$$P\left(\exists t \geq T\colon \tilde{X}_t \in \mathcal{X}_u\right) \leq P\left(\sup_{t\geq T} V\left(\tilde{X}_t\right) \geq l\right) \leq \frac{E[V(X_0)]}{\mathrm{e}^{\Lambda T} l}.$$

This completes the proof. □

Now we lift the results to the slightly more involved case with $m > 1$.

Proposition 2. *Suppose there exists an essentially non-negative matrix $\Lambda \in \mathbb{R}^{m\times m}$ and an m-dimensional polynomial function $V\colon \mathbb{R}^n \to \mathbb{R}^m$ satisfying Theorem 2. If all of the eigenvalues of Λ have positive real parts, i.e.,*

$$\min_{1\leq i\leq m} \{\Re(\lambda_i) \mid \lambda_i \text{ is an eigenvalue of } \Lambda\} > 0,$$

then for any positive vector $\gamma \in \mathbb{R}^m$, there exists $T^* = T^*(\gamma, M, \Lambda) \in \mathbb{R}$ such that for any $T \geq T^*$,

$$P\left(\sup_{t\geq T} V\left(\tilde{X}_t\right) \geq \gamma\right) \leq \frac{E[V_i(X_0)]}{(\mathrm{e}^{MT}\gamma)_i} \tag{10}$$

holds for all $i \in \{1, \ldots, m\}$. Here, M is an essentially non-negative matrix s.t. all of the eigenvalues of $\Lambda - M$ have positive real parts[5]. Moreover, if there exists a positive vector $l \in \mathbb{R}^m$ such that

$$V(x) \geq l \quad \text{for all } x \in \mathcal{X}_u,$$

then for any $T \geq T^*$,

$$P\left(\exists t \geq T\colon \tilde{X}_t \in \mathcal{X}_u\right) \leq \frac{E[V_i(X_0)]}{(\mathrm{e}^{MT} l)_i} \tag{11}$$

holds for all $i \in \{1, \ldots, m\}$.

Proof. By substituting γ in Eq. (7) with $\mathrm{e}^{MT}\gamma$, we have that for all $T \geq 0$,

$$\begin{aligned} \frac{E[V_i(X_0)]}{(\mathrm{e}^{MT}\gamma)_i} &\geq P\left(\sup_{t\geq T} V\left(\tilde{X}_t\right) \geq \sup_{t\geq T}\left(\mathrm{e}^{-\Lambda t}\mathrm{e}^{MT}\gamma\right)\right) \\ &= P\left(\sup_{t\geq T} V\left(\tilde{X}_t\right) \geq \sup_{t\geq T}\left(\mathrm{e}^{-\Lambda(t-T)}\mathrm{e}^{-(\Lambda-M)T}\gamma\right)\right) \end{aligned} \tag{12}$$

holds for any $\gamma \in \mathbb{R}^m$ with $\gamma > \mathbf{0}$. Observe that

$$\begin{aligned} \left|\sup_{t\geq T}\left(\mathrm{e}^{-\Lambda(t-T)}\mathrm{e}^{-(\Lambda-M)T}\gamma\right)\right|_\infty &= \left|\sup_{t\geq 0}\left(\mathrm{e}^{-\Lambda t}\mathrm{e}^{-(\Lambda-M)T}\gamma\right)\right|_\infty \\ &\leq \left|\sup_{t\geq 0}\left(\mathrm{e}^{-\Lambda t}\right)\right|_\infty \left|\mathrm{e}^{-(\Lambda-M)T}\gamma\right|_\infty, \end{aligned}$$

[5] Such matrix M always exists, for instance, $M \mathrel{\widehat{=}} \Lambda/2$.

where $|\cdot|_\infty$ denotes the infinity norm. Moreover, since all of the eigenvalues of $\Lambda - M$ have positive real parts, then by the Lyapunov stability established in the theory of ODEs, we have

$$\lim_{T\to\infty} \mathrm{e}^{-(\Lambda-M)T}\gamma = \mathbf{0}.$$

There hence exists T^* s.t. for all $T \geq T^*$,

$$\sup_{t\geq T}\left(\mathrm{e}^{-\Lambda(t-T)}\mathrm{e}^{-(\Lambda-M)T}\gamma\right) \leq \gamma. \tag{13}$$

By Combining Eq. (13) and Eq. (12), we obtain Eq. (10). For Eq. (11), it follows immediately that

$$P\left(\exists t \geq T\colon \tilde{X}_t \in \mathcal{X}_u\right) \leq P\left(\sup_{t\geq T} V\left(\tilde{X}_t\right) \geq l\right) \leq \frac{E[V_i(X_0)]}{(\mathrm{e}^{MT}l)_i}.$$

This completes the proof. □

Remark 3. Proposition 2 argues the existence of T^* that suffices to "split off" the tail failure probability. From a computational perspective, this is algorithmically tractable as the matrix exponential involved in Eq. (13) is symbolically computable (cf., e.g., [23]).

The following theorem states the main result of this section, that is, for any given constant ϵ, there exists $\tilde{T} \geq 0$ such that the truncated $\tilde{T}$-tail failure probability is bounded by ϵ:

Theorem 4. *Suppose the conditions in Proposition 1 and 2 are satisfied. If there exists $\alpha > 0$, s.t. $\forall x \in \mathcal{X}_0\colon V_i(x) \leq \alpha$ holds for some $i \in \{1,\ldots,m\}$. Then for any $\epsilon > 0$, there exists $\tilde{T} \geq 0$ such that*

$$P\left(\exists t \geq \tilde{T}\colon \tilde{X}_t \in \mathcal{X}_u\right) \leq \epsilon.$$

Proof. Observe that for Eq. (11) in Proposition 2, the assumption $\forall x \in \mathcal{X}_0\colon V_i(x) \leq \alpha$ guarantees an upper bound on the numerator $E[V_i(X_0)]$, while the essential non-negativity of M (with all its eigenvalues having positive real parts) ensures that the denominator $(\mathrm{e}^{MT}l)_i \to +\infty$ as $T \to \infty$. An analogous argument applies to Eq. (9) in Proposition 1. The claim in this theorem then follows immediately. □

3.2 Bounding the Failure Probability over $[0, T]$

The reduced T-safety problem can be solved by existing methods tailored for bounded verification of SDEs, e.g., [32,35]. In what follows, we propose an alternative method leveraging time-dependent polynomial stochastic barrier certificates. Our method requires constraints (on the barrier certificates) of simpler form compared to [35]; meanwhile, it yields strictly more expressive

form of barrier certificates, against the approach on unbounded verification as in [27,28], thus leading to theoretically non-looser (usually tighter) failure bound. A detailed argument will be given at the end of this section.

The following theorem states a sufficient condition, i.e., a collection of constraints on the time-dependent polynomial stochastic barrier certificates $H(t,x)$, under which the failure probability of a stochastic system over a finite time horizon can be explicitly bounded from above.

Theorem 5. *Suppose there exists a constant $\eta > 0$ and a polynomial function (termed* time-dependent stochastic barrier certificate*) $H(t,x)\colon \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}$, satisfying*[6]

$$H(t,x) \geq 0 \quad \textit{for } (t,x) \in [0,T] \times \mathcal{X}, \tag{14}$$

$$\mathcal{A}H(t,x) \leq 0 \quad \textit{for } (t,x) \in [0,T] \times (\mathcal{X} \setminus \mathcal{X}_u), \tag{15}$$

$$\frac{\partial H}{\partial t} \leq 0 \quad \textit{for } (t,x) \in [0,T] \times \partial\mathcal{X}, \tag{16}$$

$$H(t,x) \geq \eta \quad \textit{for } (t,x) \in [0,T] \times \mathcal{X}_u. \tag{17}$$

Then,

$$P\left(\exists t \in [0,T]\colon \tilde{X}_t \in \mathcal{X}_u\right) \leq \frac{E[H(0,X_0)]}{\eta}. \tag{18}$$

Proof. Assume in the following that the system evolves within a bounded domain $\mathcal{X}$[7]. Define a stopping time

$$\tau_u \mathrel{\widehat{=}} \inf\left\{t \mid \tilde{X}_t \notin \mathcal{X} \setminus \mathcal{X}_u\right\},$$

and denote by $X_t^{(u)} \mathrel{\widehat{=}} (t \wedge \tau_u \wedge T, \tilde{X}_{t\wedge\tau_u\wedge T})$ the corresponding stopped process, and by $\mathcal{A}^{(u)}$ the corresponding infinitesimal generator. By Eq. (3), we have

$$\begin{aligned}\mathcal{A}^{(u)}H\left(X_t^{(u)}\right) &= \mathcal{A}^{(u)}H\left(t \wedge \tau_u \wedge T, \tilde{X}_{t\wedge\tau_u\wedge T}\right)\\ &= \begin{cases} 0 & \text{if } t \geq T \vee t \geq \tau_u(\omega),\\ \mathcal{A}H(t,X_t) \leq 0 & \text{if } t < \min\{T, \tau_u(\omega), \tau_{\mathcal{X}}(\omega)\},\\ \frac{\partial H}{\partial t}(t,X_t) \leq 0 & \text{if } t < \min\{T,\tau_u(\omega)\} \wedge t \geq \tau_{\mathcal{X}}(\omega).\end{cases}\end{aligned}$$

By Dynkin's formula, for fixed $t, h \in [0,T]$, we have

$$\begin{aligned}E\left[H\left(X_{t+h}^{(u)}\right) \mid \mathcal{F}_h\right] &= E^{X_h^{(u)}}\left[H\left(X_{t+h}^{(u)}\right)\right]\\ &= E\left[H\left(X_h^{(u)}\right)\right] + E^{X_h^{(u)}}\left[\int_0^t \mathcal{A}^{(u)}H\left(X_s^{(u)}\right)\,\mathrm{d}s\right]\\ &\leq E\left[H\left(X_h^{(u)}\right)\right].\end{aligned}$$

[6] Condition (16) is to ensure that when $\tilde{X}_t$ stops at the boundary of $\mathcal{X}$, we still have $\tilde{A}H(t,x) \leq 0$ for $x \in \partial\mathcal{X}$. If $\mathcal{X} = \mathbb{R}^n$, however, this condition can be dropped.

[7] For cases with an unbounded $\mathcal{X}$, the same proof technique of introducing a δ-closed ball as in the proof of Theorem 2 applies.

Thus $H(X_t^{(u)})$ is a non-negative supermartingale. Then by Doob's maximal inequality in Lemma 3, we have

$$\begin{aligned} P\left(\exists t \in [0,T] \colon \tilde{X}_t \in \mathcal{X}_u\right) &= P\left(\exists t \geq 0 \colon \tilde{X}_{t\wedge\tau_u\wedge T} \in \mathcal{X}_u\right) \\ &\leq P\left(\exists t \geq 0 \colon H\left(X_t^{(u)}\right) \geq \eta\right) \\ &\leq \frac{E[H(0,X_0)]}{\eta}. \end{aligned}$$

This completes the proof. □

The following fact is then immediately obvious:

Corollary 1. *Suppose the conditions in Theorem 5 hold, and there exists $\beta > 0$, s.t. $H(0,x) \leq \beta$ for $x \in \mathcal{X}_0$. Then,*

$$P\left(\exists t \in [0,T] \colon \tilde{X}_t \in \mathcal{X}_u\right) \leq \frac{\beta}{\eta}.$$

Proof. This is a direct consequence of Theorem 5. □

Remarks on Potentially Tighter Bound. There exists already in the literature a barrier certificate-based method proposed in [27,28] that can deal with the ∞-safety problem. It is worth highlighting, however, that our bound on the overall failure probability derived from Proposition 1, 2 and Theorem 5 (with appropriate $\tilde{T}$ chosen) is at least as tight as (and usually tighter than, as can be seen later in the experiments) that in [27,28]. The reasons are twofold: (1) the reduction to a finite-time horizon $\tilde{T}$-safety problem substantially "trims off" verification efforts pertaining to $t > \tilde{T}$; (2) our method for the reduced $\tilde{T}$-safety problem admits time-dependent barrier certificates, which are strictly more expressive than those time-independent ones exploited in [27,28], in the sense that any feasible solution thereof shall also be a feasible solution satisfying Theorem 5.

Remark 4. Roughly speaking, by setting the diffusion coefficients σ in SDEs to zero, our method applies trivially to ODE dynamics with either a known or an unknown probability distribution over the initial set of states. For the former, we can even obtain a tighter bound on the failure probability, since in this case we do not need to compute a bound on the barrier certificate over all possible initial distributions.

4 Synthesizing Stochastic Barrier Certificates Using SDP

In this section, we encode the synthesis of the aforementioned exponential and time-dependent stochastic barrier certificates into semidefinite programming [38] optimizations, and thus a solution thereof yields an upper bound on the failure

probability over the infinite-time horizon. Specifically, an SDP problem is formulated, for each of the two barrier certificates, to encode the constraints for "being an exponential/time-dependent stochastic barrier certificate", while in the meantime optimizing the tightness of the failure probability bound.

It is worth noting that SDP is a generalization of the standard linear programming in which the element-wise non-negativity constraints are replaced by a generalized inequality w.r.t. the cone of positive semidefinite matrices. The generalization preserves *convexity*, leading to the fact that SDP admits polynomial-time algorithms, say the well-known *interior-point methods*, that can efficiently solve the synthesis problem, albeit numerically. We remark that the numerical computation employed in off-the-shelf SDP solvers and the use of interior-point algorithms may potentially lead to erroneous results and thereby unsoundness in the verification/synthesis results. There have been numerous attempts to validate the results from the solver through a-posteriori numerical verification of the solution. For more details, we refer the readers to [30] and the references therein.

Exponential Stochastic Barrier Certificate $V(x)$. To encode the synthesis problem into an SDP optimization, we first fix the dimension m together with Λ satisfying Proposition 1 or 2 (depending on m), and then assume a polynomial template $V^a(x)$ of certain degree k with unknown parameters a, as the barrier certificate to be discovered. It then suffices to solve the following SDP problem[8]:

$$\begin{aligned}
\underset{a,\alpha}{\texttt{minimize}} \quad & \alpha && (19)\\
\texttt{subject to} \quad & V^a(x) \geq \mathbf{0} \quad \text{for } x \in \mathcal{X} && (20)\\
& \mathcal{A}V^a(x) \leq -\Lambda V^a(x) \quad \text{for } x \in \mathcal{X} && (21)\\
& \Lambda V^a(x) \leq \mathbf{0} \quad \text{for } x \in \partial\mathcal{X} && (22)\\
& V^a(x) \geq \mathbf{1} \quad \text{for } x \in \mathcal{X}_u && (23)\\
& V^a(x) \leq \alpha\mathbf{1} \quad \text{for } x \in \mathcal{X}_0 && (24)
\end{aligned}$$

Here, the constraints (20)–(22) encode the definition of an exponential stochastic barrier certificate (cf. Theorem 2), while constraint (23) (resp., (24)) corresponds to the lower (resp., upper) bound of $V(x)$ as in Proposition 1 and 2 (resp., Theorem 4)[9]. Hence, minimizing the upper bound α of (each component of) $V^a(x)$ gives a tight exponentially decreasing bound on the tail failure probability, as claimed in Proposition 1 and 2.

Remark 5. If Λ is chosen as a non-negative matrix, the combination of condition (20) and (22) will force $V^a(x) = \mathbf{0}$ for $x \in \partial\mathcal{X}$, whereof the strict equality

[8] SDP problems in this paper refer to those that can be readily translated into the standard form of SDP, through, e.g., Stengle's Positivstellensatz [36] and sum-of-squares decomposition [26].

[9] The lower bound l of $V(x)$ in Proposition 1 and 2 is normalized to a vector with all its components no less than 1, based on the observation that, for any $c > 0$, $V^a(x)$ is a feasible solution implies $cV^a(x)$ is also a feasible solution.

may be violated due to numerical computations in SDP. In practice, however, this issue can be well addressed by looking for a barrier certificate of the form $g(x)V(x)$, where $g(x)$ satisfies $\partial\mathcal{X} \subseteq \{x \mid g(x) = 0\}$, namely, an overapproximation of the boundary of $\mathcal{X}$.

Remark 6. The choice of m is arbitrary, while the choices of Λ and k can be heuristic: If Λ_1 admits no feasible solution, neither will $\Lambda_2 \geq \Lambda_1$ (point-wise, with all the rest parameters fixed); similarly, if k_1 admits no feasible solution, neither will $k_2 \leq k_1$ (with all the rest parameters fixed). Therefore, one may decrease Λ (say, by a half) or increase k (say, by one) whenever a valid barrier certificate was not found.

Time-Dependent Stochastic Barrier Certificate $H(t,x)$. Given the results established in Sect. 3, the corresponding synthesis problem can be analogously encoded as the following SDP problem:

$$\underset{b,\beta}{\texttt{minimize}} \quad \beta \tag{25}$$

$$\texttt{subject to} \quad H^b(t,x) \geq 0 \quad \text{for } (t,x) \in [0,T] \times \mathcal{X} \tag{26}$$

$$\mathcal{A}H^b(t,x) \leq 0 \quad \text{for } (t,x) \in [0,T] \times (\mathcal{X} \setminus \mathcal{X}_u) \tag{27}$$

$$\frac{\partial H^b}{\partial t} \leq 0 \quad \text{for } (t,x) \in [0,T] \times \partial\mathcal{X} \tag{28}$$

$$H^b(t,x) \geq 1 \quad \text{for } (t,x) \in [0,T] \times \mathcal{X}_u \tag{29}$$

$$H^b(0,x) \leq \beta \quad \text{for } x \in \mathcal{X}_0 \tag{30}$$

Similarly, the constraints (26)–(29) encode the definition of a time-dependent stochastic barrier certificate (cf. Theorem 5), while constraint (30) corresponds to the upper bound of $H(t,x)$ as in Corollary 1 (with η being normalized to 1, as in constraint (29)). Consequently, minimizing the upper bound β of $H^b(t,x)$ produces a tight bound on the failure probability over the reduced finite-time horizon, as stated in Corollary 1.

Remark 7. The state-of-the-art interior-point methods solve an SDP problem up to an error ε in time that is polynomial in the program description size (number of variables) and $\log(1/\varepsilon)$. The former is exponential in the degree of V^a and H^b, as it corresponds to the number of monomials in the template polynomials.

5 Implementation and Experimental Results

To further demonstrate the practical performance of our approach, we have carried out a prototypical implementation in MATLAB R2019b, with the toolbox YALMIP [21] and MOSEK [2] equipped for formulating and solving the underlying SDP problems. Given an ∞-safety problem as input, our implementation works toward an upper bound on the failure probability over the infinite time

horizon, leveraging the reduction to a T-safety problem based on a computed exponentially decreasing bound on the tail failure probability. A collection of benchmark examples from the literature has been evaluated on a 1.8 GHz Intel Core-i7 processor with 8 GB RAM running 64-bit Windows 10. Each of the examples has been successfully tackled within 30 s. In what follows, we demonstrate the applicability of our techniques to SDEs featuring different dimensionalities and nonlinear dynamics, and show particularly that our approach usually produces tighter bounds compared to existing methods.

Example 1 (Population growth [25]). Consider the stochastic system

$$\mathrm{d}X_t = b\,(X_t)\;\mathrm{d}t + \sigma\,(X_t)\;\mathrm{d}W_t,$$

which is a stochastic model of population dynamics subject to random fluctuations that, possibly, can be attributed to extraneous or chance factors such as the weather, location, and the general environment. Suppose that the state space is restricted within $\mathcal{X} = \{x \mid x \geq 0\}$ with $b(X_t) = -X_t$ and $\sigma(X_t) = \sqrt{2}/2X_t$. We instantiate the ∞-safety problem as $\mathcal{X}_0 = \{x \mid x = 1\}$ and $\mathcal{X}_u = \{x \mid x \geq 2\}$, namely, we expect that the population does not diverge beyond 2.

Let $\Lambda = 1$ (with $m = 1$) and set the polynomial template degree of the exponential stochastic barrier certificate $V^a(x)$ to 4, the SDP solver gives

$$\begin{aligned} V^a(x) = {} & 0.000001474596322 - 0.000044643990040x \\ & + 0.125023372121222x^2 + 0.000000001430428x^3, \end{aligned}$$

which satisfies

$$V^a(x) \geq 1 \;\text{ for } x \in \mathcal{X}_u \quad \text{and} \quad V^a(x) \leq 0.12498 \;\text{ for } x \in \mathcal{X}_0.$$

Thus by Proposition 1, we obtain the exponentially decreasing bound

$$P\left(\exists t \geq T\colon \tilde{X}_t \in \mathcal{X}_u\right) \leq \frac{0.12498}{\mathrm{e}^T} \quad \text{for all } T > 0.$$

The user then may choose any $T > 0$ and solve the reduced T-safety problem. As depicted in the left of Fig. 1, different choices lead to different bounds on the failure probability. Nevertheless, one may surely select an appropriate T that yields a way tighter overall bound on the failure probability than that produced by the method in [27,28].

Example 2 (Harmonic oscillator [13]). Consider a two-dimensional harmonic oscillator with noisy damping:

$$\mathrm{d}X_t = \begin{pmatrix} 0 & \omega \\ -\omega & -k \end{pmatrix} X_t\;\mathrm{d}t + \begin{pmatrix} 0 & 0 \\ 0 & -\sigma \end{pmatrix} X_t\;\mathrm{d}W_t,$$

with constants $\omega = 1, k = 7$ and $\sigma = 2$. We instantiate the ∞-safety problem as $\mathcal{X} = \mathbb{R}^n$, $\mathcal{X}_0 = \{(x_1, x_2) \mid -1.2 \leq x_1 \leq 0.8, -0.6 \leq x_2 \leq 0.4\}$ and $\mathcal{X}_u = \{(x_1, x_2) \mid |x_1| \geq 2\}$.

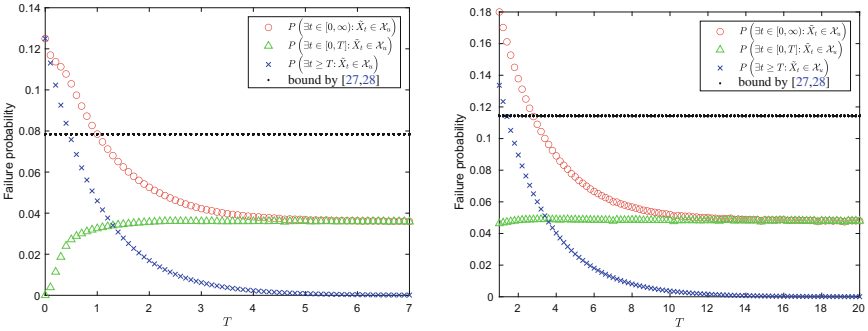

Fig. 1. Different choices of T lead to different bounds on the failure probability (with the time-dependent stochastic barrier certificates of degree 4). Note that '$\circ$' = '$\times$' + '$\triangle$' and '$\bullet$' depicts the overall bound on the failure probability produced by the method in [27,28].

Let $\Lambda = \begin{pmatrix} 0.45 & 0.1 \\ 0.1 & 0.45 \end{pmatrix}$ and set the polynomial template degree of the exponential stochastic barrier certificate $V^a(x)$ to 4, the SDP solver produces a two-dimensional $V^a(x)$ (abbreviated for clear presentation) satisfying

$$V^a(x) \le \begin{pmatrix} 0.19946 \\ 0.19946 \end{pmatrix} \quad \text{for } x \in \mathcal{X}_0 \quad \text{and} \quad V^a(x) \ge l = \begin{pmatrix} 1.000237 \\ 1.000236 \end{pmatrix} \quad \text{for } x \in \mathcal{X}_u.$$

According to the proof of Proposition 2, we set $M = \begin{pmatrix} 0.3 & 0.1 \\ 0.1 & 0.3 \end{pmatrix}$ and aim to find $T^* \ge 0$ such that for all $T \ge T^*$,

$$\sup_{t \ge 0} \left(\mathrm{e}^{-\Lambda t} \mathrm{e}^{-(\Lambda - M)T} \begin{pmatrix} 1.000237 \\ 1.000236 \end{pmatrix} \right) \le \begin{pmatrix} 1.000237 \\ 1.000236 \end{pmatrix}. \tag{31}$$

Symbolic computation on the matrix exponential gives

$$\begin{aligned} \sup_{t \ge 0} \left(\mathrm{e}^{-\Lambda t} \mathrm{e}^{-(\Lambda - M)T} \begin{pmatrix} 1.000237 \\ 1.000236 \end{pmatrix} \right) &= \sup_{t \ge 0} \begin{pmatrix} \mathrm{e}^{-0.15T}(1.0002365\mathrm{e}^{-0.55t} + 0.0000005\mathrm{e}^{-0.35t}) \\ \mathrm{e}^{-0.15T}(1.0002365\mathrm{e}^{-0.55t} - 0.0000005\mathrm{e}^{-0.35t}) \end{pmatrix} \\ &\le \begin{pmatrix} 1.0002365\mathrm{e}^{-0.15T} \\ 1.0002365\mathrm{e}^{-0.15T} \end{pmatrix}. \end{aligned}$$

Therefore, $T^* = 1$ satisfies condition (31). Further by Corollary 2, for any $T \ge T^* = 1$, we have

$$P\left(\exists t \ge T \colon \tilde{X}_t \in \mathcal{X}_u\right) \le \frac{E[V_1(X_0)]}{(\mathrm{e}^{MT} l)_1} \le \frac{0.19946}{0.0000005\mathrm{e}^{0.2T} + 1.00024\mathrm{e}^{0.4T}}.$$

Analogously, a comparison with existing methods concerning the tightness of the synthesized failure probability bound (under different choices of T) is shown in the right of Fig. 1.

Example 3 (Nonlinear drift [27]). We consider in this example a stochastic system involving nonlinear dynamics in its drift coefficient:

$$\begin{aligned} \mathrm{d}x_1(t) &= x_2(t)\ \mathrm{d}t \\ \mathrm{d}x_2(t) &= -x_1(t) - x_2(t) - 0.5x_1^3(t)\ \mathrm{d}t + 0.1\ \mathrm{d}W_t. \end{aligned}$$

As in [27], let $\mathcal{X} = \{(x_1, x_2) \mid |x_1| \leq 3, |x_2| \leq 3, x_1^2 + x_2^2 \geq 0.5^2\}$, $\mathcal{X}_0 = \{(x_1, x_2) \mid (x_1 + 2)^2 + x_2^2 \leq 0.1^2\}$ and $\mathcal{X}_u = \{(x_1, x_2) \in \mathcal{X} \mid x_2 \geq 2.25\}$. With $\Lambda = 1.5$ $(m = 1)$, we obtain an exponential stochastic barrier certificate $V^a(x)$ of degree 8 satisfying

$$V^a(x) \leq 4.00014 \quad \text{for } x \in \mathcal{X}_0 \quad \text{and} \quad V^a(x) \geq 1.05248 \quad \text{for } x \in \mathcal{X}_u.$$

Thus by Corollary 1, we have for any $T \geq 0$,

$$P\left(\exists t \geq T\colon \tilde{X}_t \in \mathcal{X}_u\right) \leq \frac{3.80070}{\mathrm{e}^{1.5T}}.$$

Setting, for instance, $T = 6$, we have

$$P\left(\exists t \geq 0\colon \tilde{X}_t \in \mathcal{X}_u\right) \leq P\left(\exists t \in [0, 6]\colon \tilde{X}_t \in \mathcal{X}_u\right) + \frac{3.80070}{\mathrm{e}^{9}}.$$

For the reduced T-safety problem with $T = 6$, a time-dependent stochastic barrier certificate of degree 8 is synthesized, thereby yielding $P\left(\exists t \in [0, 6]\colon \tilde{X}_t \in \mathcal{X}_u\right) \leq 0.196124$, thus together we get

$$P\left(\exists t \geq 0\colon \tilde{X}_t \in \mathcal{X}_u\right) \leq 0.196593,$$

which is tighter than 0.265388 produced (on the same machine) by the method in [27] under the same template degree.

6 Conclusion

We proposed a constructive method, based on the synthesis of stochastic barrier certificates, for computing an exponentially decreasing upper bound, if existent, on the tail probability that an SDE system violates a given safety specification. We showed that such an upper bound facilitates a reduction of the verification problem over an unbounded temporal horizon to that over a bounded one. Preliminary experimental results on a set of interesting examples from the literature demonstrated the effectiveness of the reduction and that our method often produces tighter bounds on the failure probability.

For future work, we plan to investigate a possible convergence result in the sense that the derived failure probability bound may converge to the exact one as increasing the degree of the barrier certificates. Extending our technique to tackle SDEs with control inputs will also be of interest. Moreover, checking whether a given parametric (polynomial) formula keeps probabilistic invariance

plays a central in the verification of SDEs. Several kinds of sufficient conditions on probabilistic barrier certificates were proposed, including the ones given in this paper. It consequently deserves to investigate a necessary and sufficient condition for checking the probabilistic invariance of a given template, like for ODEs in [19]. Apart from that, we are interested in carrying our results to the verification of probabilistic programs without conditioning, which can be viewed as discrete-time stochastic dynamics.

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Widest Paths and Global Propagation in Bounded Value Iteration for Stochastic Games

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Abstract. Solving *stochastic games* with the reachability objective is a fundamental problem, especially in quantitative verification and synthesis. For this purpose, *bounded value iteration (BVI)* attracts attention as an efficient iterative method. However, BVI's performance is often impeded by costly *end component (EC) computation* that is needed to ensure convergence. Our contribution is a novel BVI algorithm that conducts, in addition to local propagation by the Bellman update that is typical of BVI, *global* propagation of upper bounds that is not hindered by ECs. To conduct global propagation in a computationally tractable manner, we construct a weighted graph and solve the *widest path problem* in it. Our experiments show the algorithm's performance advantage over the previous BVI algorithms that rely on EC computation.

1 Introduction

1.1 Stochastic Game (SG)

A *stochastic game* [13] is a two-player game played on a graph. In an SG, an action a of a player causes a transition from the current state s to a successor s', with the latter chosen from a prescribed probability distribution $\delta(s, a, s')$. Under the reachability objective, the two players (called *Maximizer* and *Minimizer*) aim to maximize and minimize, respectively, the reachability probability to a designated target state.

Stochastic games are a fundamental construct in theoretical computer science, especially in the analysis of probabilistic systems. Its complexity is interesting in its own: the problem of threshold reachability—whether Maximizer has a strategy that ensures the reachability probability to be at least given p—is known

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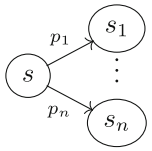
to be in UP ∩ coUP [19], but no polynomial algorithm is known. The practical significance of SGs comes from the number of problems that can be encoded to SGs and then solved. Examples include the following: solving deterministic parity games [8], solving stochastic games with the parity or mean-payoff objective [1], and a variety of probabilistic verification and reactive synthesis problems in different application domains such as cyber-physical systems. See e.g. [25].

SGs are often called 2.5-player games, where probabilistic branching is counted as 0.5 players. They generalize deterministic automata (0-player), Markov chains (MCs, 0.5-player), nondeterministic automata (1-player), Markov decision processes (MDPs, 1.5-player) and (deterministic) games (2-player). Many theoretical considerations on these special cases carry over smoothly to SGs. However, SGs have their peculiarities, too. One example is the treatment of end components in bounded value iteration, as we describe later.

1.2 Value Iteration (VI)

In an SG, we are interested in the *optimal* reachability probability, that is, the reachability probability when both Maximizer and Minimizer take their optimal strategies. The function that returns these optimal reachability probabilities is called the *value function* $V(\mathcal{G})$ of the SG $\mathcal{G}$; our interest is in computing this value function, desirably constructing optimal strategies for the two players at the same time. For this purpose, two principal families of solution methods are *strategy iteration (SI)* [19] and *value iteration (VI)* [10,13]—the latter is commonly preferred for performance reasons.

The mathematical principle that underpins VI is the characterization of the value function $V(\mathcal{G})$ as the *least fixed point (lfp)* of an function update operator $\mathbb{X}$ called the *Bellman operator*. The Bellman operator $\mathbb{X}$ back-propagates function values by one step, using the average. For the simple case of Markov chains shown on the right, it is defined by $(\mathbb{X}f)(s) = \sum_i p_i \cdot f(s_i)$, turning a function $f\colon S \to [0,1]$ (i.e., assignment of "scores" to states) to $\mathbb{X}f\colon S \to [0,1]$.



Since $V(\mathcal{G})$ is the lfp $\mu\mathbb{X}$, Kleene's fixed point theorem tells us the sequence

$$\bot \;\leq\; \mathbb{X}\bot \;\leq\; \mathbb{X}^2\bot \;\leq\; \cdots, \tag{1}$$

where $\bot$ is the least element of the function space $S \to [0,1]$, converges to $V(\mathcal{G}) = \mu\mathbb{X}$. VI consists of the iterative approximation of $V(\mathcal{G})$ via the sequence (1).

An issue from the practical point of view, however, is that $\mathbb{X}^i\bot$ never becomes equal to $V(\mathcal{G})$ in general. Even worse, one cannot know how close the current approximant $\mathbb{X}^i\bot$ is to the desired function $V(\mathcal{G})$ [18]. In summary, VI as an iterative approximation method does not give any precision guarantee.

1.3 Bounded Value Iteration (BVI) and End Components

Bounded value iteration (BVI) has been actively studied as an extension of VI that comes with a precision guarantee [2,3,5,16,18,20,23]. Its core ideas are the following two.

Firstly, BVI computes not only iterative lower bounds $L_i = \mathbb{X}^i \bot$ for $V(\mathcal{G})$, but also iterative *upper bounds* U_i, as shown on the right in (2). This gives us a precision guarantee—$V(\mathcal{G})$ must lie between the approximants L_i and U_i.

$$\begin{array}{ccccccc} L_0 & \leq & L_1 & \leq & \cdots & & \\ & & & & & \searrow\!\nearrow & V(\mathcal{G}) \\ U_0 & \geq & U_1 & \geq & \cdots & \nearrow\!\searrow & \end{array} \tag{2}$$

Secondly, for computing upper bounds U_i, BVI uses the Bellman operator again: $U_i = \mathbb{X}^i \top$ where $\top$ is the greatest element of the function space $S \to [0,1]$. This leads to the following approximation sequence that is dual to (1):

$$\top \ \geq \ \mathbb{X}\top \ \geq \ \mathbb{X}^2\top \ \geq \ \cdots . \tag{3}$$

The sequence (3) converges to the *greatest fixed point (gfp)* $\nu\mathbb{X}$ of $\mathbb{X}$, which must be above the lfp $V(\mathcal{G}) = \mu\mathbb{X}$. Therefore the elements in (3) are all above $V(\mathcal{G})$.

The problem, however, is that the gfp $\nu\mathbb{X}$ is not necessarily the same as $\mu\mathbb{X}$. Therefore the upper bounds $U_0 \geq U_1 \geq \cdots$ given by (3) may not converge to $V(\mathcal{G})$. In other words, for a given threshold $\varepsilon > 0$, the bounds in (2) may fail to achieve $U_i - L_i \leq \varepsilon$, no matter how large i is.

In the literature, the source of this convergence issue has been identified to be *end components (ECs)* in MCs/MDPs/SGs. ECs are much like loops without exits—an example is in Fig. 1, where we use a Markov chain (MC) for simplicity. Any function f that assigns the same value to the states s_I and s can be a fixed point of the Bellman operator $\mathbb{X}$ (that back-propagates f by averages); therefore, the gfp $\nu\mathbb{X}$ assigns 1 to both s_I and s. In contrast, $(\mu\mathbb{X})(s_I) = (\mu\mathbb{X})(s) = 0$, which says one never reaches the target $\mathbf{1}$ from s_I or s (which is obvious).

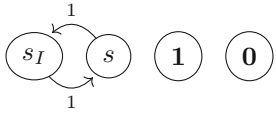


Fig. 1. A Markov chain (MC) for which the naive BVI fails to converge

Most previous works on BVI have focused on the problem of how to deal with ECs. Their solutions are to get somehow rid of ECs. For example, ECs in MDPs are discovered and *collapsed* in [5,18]; ECs in SGs cannot simply be collapsed, and an elaborate method is proposed in the recent work [20] that *deflates* them. This is the context of the current work, and we aim to enhance BVI for SGs.

1.4 Contribution: Global Propagation in BVI with Widest Paths

The algorithms in [20] seem to be the only BVI algorithms known for SGs. In their performance, however, EC computation often becomes a bottleneck. Our contribution in this paper is a new BVI algorithm for SGs that is *free from the need for EC computation*.

The key idea of our algorithm is *global propagation* for upper bounds, as sketched below. In each iteration for upper bounds $U_0 \geq U_1 \geq \cdots$, we conduct *global* propagation, in addition to the *local* propagation in the usual BVI. The latter means the application of $\mathbb{X}$ to $\mathbb{X}^i\top$, leading to $\mathbb{X}^{i+1}\top$; this local propagation, as we previously discussed, gets trapped in end components. In contrast, our global propagation looks at paths from each state s to the target $\mathbf{1}$, ignoring end components. For example, in Fig. 1, our global propagation sees that there

is no path from s_I to the target $\mathbf{1}$, and consequently assigns 0 as an upper bound for the value function $V(\mathcal{G})(s_I)$.

Such global propagation is easier said than done—in fact, the very advantage of VI is that the *global* quantities (namely reachability probabilities) get computed by iterations of *local* propagation. Conducting global propagation in a computationally tractable manner requires a careful choice of its venue. The solution in this paper is to compute *widest paths* in a suitable (directed) weighted graph.

More specifically, in each iteration where we compute an upper bound U_i, we conduct the following operations.

- (Player reduction) We turn the given SG $\mathcal{G}$ into an MDP $\mathcal{M}_i$, by restricting Minimizer's actions to the *empirically optimal* ones. The latter means they are optimal with respect to the current under-approximation L_i of $V(\mathcal{G})$.
- (Local propagation) The MDP $\mathcal{M}_i$ is then turned into a weighted graph (WG) $\mathcal{W}_i$. The construction of $\mathcal{W}_i$ consists of the application of $\mathbb{X}$ to the previous bound U_{i-1} (i.e. local propagation), and forgetting the information that cannot be expressed in a weighted graph (such as the precise transition probabilities $\delta(s, a, s')$ that depend on the action a).
  Due to this information loss, our analysis in $\mathcal{W}_i$ is necessarily approximate. Nevertheless, the benefit of $\mathcal{W}_i$'s simplicity is significant, as in the following step.
- (Global propagation) In the WG $\mathcal{W}_i$, we solve the *widest path problem*. This classic graph-theoretic problem can be solved efficiently, e.g., by the Dijkstra algorithm. The widest path width gives a new upper bound U_i.

We prove the correctness of our algorithm: soundness ($V(\mathcal{G}) \leq U_i$), and convergence ($U_i \to V(\mathcal{G})$ as $i \to \infty$). That the upper bounds decrease ($U_0 \geq U_1 \geq \cdots$) will be obvious by construction. These correctness proofs are technically nontrivial, combining combinatorial, graph-theoretic, and analytic arguments.

We have also implemented our algorithm. Our experiments compare its performance to the algorithms from [20] (the original one and its learning-based variation). The results show our consistent performance advantage: depending on SGs, our performance is from comparable to dozens of times faster. The advantage is especially eminent in SGs with many ECs.

1.5 Related Works

VI and BVI have been pursued principally for MDPs. The only work we know that deals with SGs is [20]—with the exception of [26] that works in a restricted setting where every end component belongs exclusively to either player. The work closest to ours is therefore [20], in that we solve the same problem.

For MDPs, the idea of BVI is first introduced in [23]; they worked in a limited setting where ECs do not cause the convergence issue. Its extension to general MDPs with the reachability objective is presented in [5,18], where ECs are computed and then collapsed. BVI is studied under different names in these

works: *bounded real time dynamic programming* [5,23] and *interval iteration* [18]. The work [20] is an extension of this line of work from MDPs to SGs.

The work [20] has seen a few extensions to more advanced settings: black-box settings [3], concurrent reachability [16], and generalized reachability games [2].

Most BVI algorithms involve EC computation (although ours does not). The EC algorithm in [14,15] is used in [18,20]; more recent algorithms include [7,9].

1.6 Organization

In Sect. 2 we present some preliminaries. In Sect. 3 we review VI and BVI with an emphasis on the role of Kleene's fixed point theorem. This paves the way to Sect. 4 where we present our algorithm. We do so in three steps, and prove the correctness—soundness and convergence—in the end. Experiment results are shown in Sect. 5.

2 Preliminaries

We fix some basic notations. Let X be a set. We let X^* denote the set of finite sequences over X, that is, $X^* = \bigcup_{i\in\mathbb{N}} X^i$. We let $X^+ = X^* \setminus \{\varepsilon\}$, where ε denotes the empty sequence (of length 0). The set of infinite sequences over X is denoted by X^ω. The set of functions from X to Y is denoted by $X \to Y$.

2.1 Stochastic Games

In a stochastic game, two players (*Maximizer* $\Box$ and *Minimizer* $\bigcirc$) play against each other. The goals of the two players are to maximize and minimize the *value function*, respectively. Many different definitions are possible for value functions. In this paper (as well as all the works on (bounded) value iteration), we focus on the *reachability objective*, in which case a value function is defined by the reachability probability to a designated target state $\mathbf{1}$.

Definition 2.1 (stochastic game (SG)). A stochastic game (SG) is a tuple $\mathcal{G} = (S, S_\Box, S_\bigcirc, s_I, \mathbf{1}, \mathbf{0}, A, \mathrm{Av}, \delta)$ where

- S is a finite set of *states*, partitioned into $S_\Box$ and $S_\bigcirc$ (i.e., $S = S_\Box \cup S_\bigcirc$, $S_\Box \cap S_\bigcirc = \emptyset$). $s \in S_\Box$ is *Maximizer's* state; $s \in S_\bigcirc$ is *Minimizer's* state.
- $s_I \in S$ is an *initial* state, $\mathbf{1} \in S_\Box$ is a *target*, and $\mathbf{0} \in S_\bigcirc$ is a sink.
- A is a finite set of *actions*.
- $\mathrm{Av} : S \to 2^A$ defines the set of actions that are *available* at each state $s \in S$.
- $\delta : S \times A \times S \to [0,1]$ is a *transition function*, where $\delta(s,a,s')$ gives a probability with which to reach the state s' when the action a is taken at the state s. The value $\delta(s,a,s')$ is non-zero only if $a \in \mathrm{Av}(s)$; it must satisfy $\sum_{s'\in S} \delta(s,a,s') = 1$ for all $s \in S$ and $a \in \mathrm{Av}(s)$.

We assume that each of **1** and **0** allows only one action that leads to a self-loop with probability 1. Moreover, for theoretical convenience, we assume that all SGs are non-blocking. That is, $\mathrm{Av}(s) \neq \emptyset$ for each $s \in S$.

We introduce some notations: $\mathrm{post}(s,a) = \{s' \mid \delta(s,a,s') > 0\}$, and for $S' \subseteq S$, we let $S'_\square = S' \cap S_\square$ and $S'_\bigcirc = S' \cap S_\bigcirc$.

Definition 2.2 (Markov decision process (MDP), Markov chain (MC)). An SG such that $S_\square = S \setminus \{\mathbf{0}\}$ (i.e. Minimizer is absent) is called a *Markov decision process (MDP)*. We often omit the second and third components for MDPs, writing $\mathcal{M} = (S, s_I, \mathbf{1}, \mathbf{0}, A, \mathrm{Av}, \delta)$.

An SG such that $|\mathrm{Av}(s)| = 1$ for each $s \in S$—both Maximizer and Minimizer are absent—is called a *Markov chain (MC)*. It is also denoted simply by a tuple $\mathcal{G} = (S, s_I, \mathbf{1}, \mathbf{0}, \delta)$ where its transition function is of the type $\delta : S \times S \to [0,1]$.

Every notion for SGs that appears below applies to MDPs and MCs, too.

Example 2.3. Figure 2 presents an example of an SG. At the state s_1 of Minimizer, two actions α and β are in $\mathrm{Av}(s_1)$. If Minimizer chooses α, the next state is s_2 with probability $\delta(s_1, \alpha, s_2) = 1$. If Minimizer instead chooses β, the next state is **1** with probability $\delta(s_1, \beta, \mathbf{1}) = 0.8$ or **0** with probability $\delta(s_1, \beta, \mathbf{0}) = 0.2$.

Maximizer's goal is to reach **1** as often as possible by choosing suitable actions. Minimizer's goal is to avoid reaching **1**—this can be achieved, for example but not exclusively, by reaching **0**.

Both players choose their actions according to their *strategies*. It is well-known [13] that *positional* (also called *memoryless*) and *deterministic* (also called *pure*) strategies are complete for finite SGs with the reachability objective.

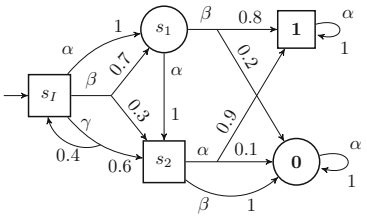


Fig. 2. A stochastic game (SG), an example

Definition 2.4 (strategy, path). Let $\mathcal{G}$ be the SG in Definition 2.1. A *strategy* for Maximizer in $\mathcal{G}$ is a function $\sigma \colon S_\square \to A$ such that $\sigma(s) \in \mathrm{Av}(s)$ for each $s \in S_\square$. A *strategy* for Minimizer is defined similarly. The set of Maximizer's strategies in $\mathcal{G}$ is denoted by $\mathrm{str}^{\mathcal{G}}_\square$; that of Minimizer's is denoted by $\mathrm{str}^{\mathcal{G}}_\bigcirc$.

Strategies $\tau \in \mathrm{str}^{\mathcal{G}}_\square$ and $\sigma \in \mathrm{str}^{\mathcal{G}}_\bigcirc$ in $\mathcal{G}$ turn the game $\mathcal{G}$ into a Markov chain, which is denoted by $\mathcal{G}^{\tau,\sigma}$. Similarly, a strategy τ for Maximizer (who is the only player) in an MDP $\mathcal{M}$ induces an MC, denoted by $\mathcal{M}^\tau$.

An *infinite path* in $\mathcal{G}$ is a sequence $s_0 a_0 s_1 a_1 s_2 a_2 \ldots \in (S \times A)^\omega$ such that for all $i \in \mathbb{N}$, $a_i \in \mathrm{Av}(s_i)$ and $s_{i+1} \in \mathrm{post}(s_i, a_i)$. A prefix $s_0 a_0 s_1 \ldots s_k$ of an infinite path ending with a state is called a *finite path*. If $\mathcal{G}$ is an MC, then we omit actions in a path and write $s_0 s_1 s_2 \ldots$ or $s_0 s_1 \ldots s_k$.

Given a game $\mathcal{G}$ and strategies τ, σ for the two players, the induced MC $\mathcal{G}^{\tau,\sigma}$ assigns to each state $s \in S$ a probability distribution $\mathbb{P}^{\tau,\sigma}_s$. The distribution is with respect to the standard measurable structure of S^ω; see, e.g., [4, Chap. 10].

For each measurable subset $X \subseteq S^\omega$, $\mathbb{P}_s^{\tau,\sigma}(X)$ is the probability with which $\mathcal{G}^{\tau,\sigma}$, starting from the state s, produces an infinite path π that belongs to X.

It is well-known that all the LTL properties are measurable in S^ω. In the current setting with the reachability objective, we are interested in the probability of eventually reaching $\mathbf{1}$, denoted by $\mathbb{P}_s^{\tau,\sigma}(\Diamond \mathbf{1})$.

Definition 2.5 (value function $V(\mathcal{G})$). Let $\mathcal{G}$ be the SG in Definition 2.1. The *value function* $V(\mathcal{G})$ of $\mathcal{G}$ is defined by

$$V(\mathcal{G})(s) = \max_{\tau \in \mathrm{str}_\Box^{\mathcal{G}}} \min_{\sigma \in \mathrm{str}_\bigcirc^{\mathcal{G}}} \mathbb{P}_s^{\tau,\sigma}(\Diamond \mathbf{1}) = \min_{\sigma \in \mathrm{str}_\bigcirc^{\mathcal{G}}} \max_{\tau \in \mathrm{str}_\Box^{\mathcal{G}}} \mathbb{P}_s^{\tau,\sigma}(\Diamond \mathbf{1}),$$

where the last equality is shown in [13].

We say a strategy τ of Maximizer's is *optimal* if $V(\mathcal{G})(s) = \min_\sigma \mathbb{P}_s^{\tau,\sigma}(\Diamond \mathbf{1})$ for each $s \in S$; similarly, we say a strategy σ of Minimizer's is *optimal* if $V(\mathcal{G})(s) = \max_\sigma \mathbb{P}_s^{\sigma,\tau}(\Diamond \mathbf{1})$ for each $s \in S$.

We write V for $V(\mathcal{G})$ when the dependence on $\mathcal{G}$ is clear from the context.

The set of states with a non-zero value is denoted by $S_{\Diamond \mathbf{1}}$. That is, $S_{\Diamond \mathbf{1}} = \{s \in S \mid V(\mathcal{G})(s) > 0\}$.

Example 2.6. Consider the SG $\mathcal{G}$ from Fig. 2. At s_2, Maximizer's action should be α. Hence, $V(\mathcal{G})(s_2) = 0.9$. At s_1, if Minimizer chooses α, then the probability of reaching $\mathbf{1}$ will be 0.9 by $V(\mathcal{G})(s_2)$. Thus, Minimizer should choose β at s_1, which yields $V(\mathcal{G})(s_1) = 0.8$. Finally, at s_I, γ is the best choice, since Maximizer can choose this action infinitely often until it gets to s_2. We have $V(\mathcal{G})(s_I) = 0.9$.

2.2 The Widest Path Problem

Definition 2.7 (weighted graph (WG)). A (directed) *weighted graph* is a triple $\mathcal{W} = (V, E, w)$ of a finite set V of *vertices*, a set $E \subseteq V \times V$ of *edges*, and a *weight function* $w \colon E \to [0, 1]$ where $[0, 1]$ is the unit interval.

A (finite) *path* in a WG is defined in the usual graph-theoretic way.

In the widest path problem, an edge weight $w(v, v')$ is thought of as its capacity, and the capacity of a path is determined by its bottleneck. The problem asks for a path with the greatest capacity. In this paper, we use the following *all-source single-destination* version of the problem.

Definition 2.8 (the widest path problem (WPP)). A (finite) *path* in $\mathcal{W} = (V, E, w)$ is a sequence $v_0 v_1 \dots v_n$ of vertices such that $(v_i, v_{i+1}) \in E$ for each $i \in [0, n-1]$. The *width* of a path $v_0 v_1 \dots v_n$ is given by $\min_{i \in [0,n-1]} w(v_i, v_{i+1})$.

The *widest path problem* is the following problem.

Given: a WG $\mathcal{W} = (V, E, w)$ and a target vertex $v_\mathrm{t} \in V$.
Answer: for each $v \in V$, the widest width of the paths from v to v_t, that is,

$$\max_{n \in \mathbb{N}, v = v_0, v_1, \dots, v_n = v_\mathrm{t}} \min_{i \in [0,n-1]} w(v_i, v_{i+1}),$$

We let $\mathrm{WPW}(\mathcal{W}, v_\mathrm{t})$ denote a function that solves this problem, and let $\mathrm{WPath}(\mathcal{W}, v_\mathrm{t})$ denote a function that assigns to each $v \in V$ a widest path to v_t. Furthermore, we assume the following property of WPath: if $\mathrm{WPath}(\mathcal{W}, v_\mathrm{t})(v_0) = v_0 v_1 \dots v_k v_\mathrm{t}$, then $\mathrm{WPath}(\mathcal{W}, v_\mathrm{t})(v_i) = v_i v_{i+1} \dots v_k v_\mathrm{t}$ for each $i \in [0, k]$.

Efficient algorithms are known for $\mathrm{WPW}(\mathcal{W}, v_\mathrm{t})$. An example is the Dijkstra search algorithm with Fibonacci heaps [17]; it is originally for the single-source all-destination version but its adaptation is easy. The algorithm runs in time $O(|E| + |V| \log |V|)$. It returns a widest path in addition to its width, too, computing the function $\mathrm{WPath}(\mathcal{W}, v_\mathrm{t})$ with the property required in the above.

3 (Bounded) Value Iteration

3.1 Bellman Operator and Value Iteration

The following construct—used for "local propagation" in computing the value function—is central to formal analysis of probabilistic systems and games.

Definition 3.1 (Bellman Operator). Let $\mathcal{G} = (S, S_\Box, S_\bigcirc, s_I, \mathbf{1}, \mathbf{0}, A, \mathrm{Av}, \delta)$ be a stochastic game. For each state $s \in S$, an available action $a \in \mathrm{Av}(s)$, and $f : S \to [0, 1]$, we define a function $\mathbb{X}_a f : S \to [0, 1]$ by the following.

$$(\mathbb{X}_a f)(s) = \begin{cases} 1 & \text{if } s = \mathbf{1}, \\ 0 & \text{if } s = \mathbf{0}, \\ \sum_{s' \in S} \delta(s, a, s') \cdot f(s') & \text{if } s \neq \mathbf{0}, \mathbf{1}. \end{cases}$$

These functions are used in the following definition of the *Bellman operator* $\mathbb{X}\colon (S \to [0, 1]) \to (S \to [0, 1])$ over $\mathcal{G}$:

$$(\mathbb{X} f)(s) = \begin{cases} \max_{a \in \mathrm{Av}(s)} (\mathbb{X}_a f)(s) & \text{if } s \in S_\Box \text{ is a Maximizer state}, \\ \min_{a \in \mathrm{Av}(s)} (\mathbb{X}_a f)(s) & \text{if } s \in S_\bigcirc \text{ is a Minimizer state}. \end{cases}$$

The function space $S \to [0, 1]$ inherits the usual order $\leq$ between real numbers in the unit interval $[0, 1]$, that is, $f \leq g$ if $f(s) \leq g(s)$ for each $s \in S$. The Bellman operator $\mathbb{X}$ over $S \to [0, 1]$ is clearly monotone; it is easily seen to preserve max and min, using the fact that the state space S of an SG is finite. Therefore we obtain the following, as consequences of Kleene's fixed point theorem.

Lemma 3.2. *Assume the setting of Definition 3.1.*

1. *The Bellman operator $\mathbb{X}$ has the greatest fixed point (gfp) $\nu\mathbb{X}\colon S \to [0, 1]$. It is obtained as the limit of the descending ω-chain*

$$\top \geq \mathbb{X}\top \geq \mathbb{X}^2\top \geq \cdots,$$

where $\top$ is the greatest element of $S \to [0, 1]$ (i.e., $\top(s) = 1$ for each $s \in S$). In other words, we have $(\nu\mathbb{X})(s) = \inf_{i \in \mathbb{N}} \big((\mathbb{X}^i \top)(s)\big)$ for each $s \in S$.

Algorithm 1: Value iteration (VI) for a stochastic game $\mathcal{G} = (S, S_\Box, S_\bigcirc, s_I, \mathbf{1}, \mathbf{0}, A, \mathrm{Av}, \delta)$ and a stopping threshold $\Delta > 0$

```
1 procedure VI(G, Δ)
2     L_0 ← ⊥                                   // Initialize lower bound
3     while L_i(s_I) − L_{i−1}(s_I) < Δ do      // Typical stopping criterion
4         i++
5         L_i ← 𝕏L_{i−1}                        // Bellman update
6     return L_i(s_I)
```

2. *Symmetrically,* $\mathbb{X}$ *has the least fixed point (lfp)* $\mu\mathbb{X}\colon S \to [0,1]$*, obtained as the limit of the ascending chain*

$$\bot \leq \mathbb{X}\bot \leq \mathbb{X}^2\bot \leq \cdots, \tag{4}$$

where $\bot(s) = 0$ *for each* $s \in S$*. That is, we have* $(\mu\mathbb{X})(s) = \sup_{i\in\mathbb{N}}\big((\mathbb{X}^i\bot)(s)\big)$ *for each* $s \in S$*.* □

The following characterization is fundamental. See, e.g., [10].

Theorem 3.3. *Let* $\mathcal{G}$ *be a stochastic game. The value function* $V = V(\mathcal{G})$ *(Definition 2.5) coincides with the least fixed point* $\mu\mathbb{X}$*.* □

The fact that $V(\mathcal{G})$ is the least fixed point of $\mathbb{X}$ implies the following: a strategy τ of Maximizer is optimal if and only if $\big(\mathbb{X}_{\tau(s)}\big(V(\mathcal{G})\big)\big)(s) = V(\mathcal{G})(s)$ holds for each $s \in S_\Box$; similarly for Minimizer. We say $a \in \mathrm{Av}(s)$ is *optimal* at s if $\mathbb{X}_a V(\mathcal{G})(s) = V(\mathcal{G})(s)$ holds; otherwise a is *suboptimal*.

Lemma 3.2.2 & Theorem 3.3 suggest iterative *under*-approximation of $V(\mathcal{G})$ by $\bot \leq \mathbb{X}\bot \leq \mathbb{X}^2\bot \leq \cdots$. This is the principle of *value iteration* (VI); see Algorithm 1.

Example 3.4. The values L_i computed by Algorithm 1, for the SG in Fig. 2, are shown in the following table. The values at $\mathbf{0}$ and $\mathbf{1}$ are omitted.

s	L_0	L_1	L_2	L_3	L_4	L_5	...	$V(\mathcal{G})$
s_I	0	0	0.54	0.83	0.872	0.8888		0.9
s_1	0	0	0.8	0.8	0.8	0.8	...	0.8
s_2	0	0.9	0.9	0.9	0.9	0.9		0.9

$L_i(s_I)$ converges to, but is never equal to, $V(\mathcal{G})(s_I)$. The converges rate can be arbitrarily slow: for any $\varepsilon \in (0,1)$ and $k \in \mathbb{N}$ there is an SG $\mathcal{G}$ and a state s such that $V(\mathcal{G})(s) - L_k(s) > \varepsilon$. One sees this by modifying Fig. 2 with $\delta(s_I, \gamma, s_2) = \varepsilon'$ and $\delta(s_I, \gamma, s_I) = 1 - \varepsilon'$, where $\varepsilon' > 0$ is an arbitrary small positive constant.

Algorithm 2: Bounded value iteration (BVI) for a stochastic game $\mathcal{G} = (S, S_\Box, S_\bigcirc, s_I, \mathbf{1}, \mathbf{0}, A, \mathrm{Av}, \delta)$ and a stopping threshold $\varepsilon > 0$—a naive prototype that suffers from end components

```
1 procedure VI(𝒢, ε)
2     L_0 ← ⊥, U_0 ← ⊤                          // Initialize lower and upper bound
3     while U_i(s_I) − L_i(s_I) > ε do          // Check the gap at the initial state
4         i++
5         L_i ← 𝕏L_{i−1}, U_i ← 𝕏U_{i−1}        // Bellman update
6     return L_i(s_I)
```

There is no known stopping criterion for VI (Algorithm 1) with a precision guarantee, besides the one in [10] that is too pessimistic to be practical. The one shown in Line 3 ("little progress") is a commonly used heuristic, but it is known to lead to arbitrarily wrong results [18].

3.2 Bounded Value Iteration

When we turn back to Lemma 3.2, Lemma 3.2.1 suggests another iterative approximation, namely *over*-approximation of the value function V by $\top \geq \mathbb{X}\top \geq \mathbb{X}^2\top \geq \cdots$. The chain converges to the gfp $\nu\mathbb{X}$ that is necessarily above the lfp $\mu\mathbb{X}$. This is the principle that underlies *bounded value iteration* (BVI); see Algorithm 2 for its naive prototype. BVI has been actively studied in the literature [2,3,5,16,18,20,23], sometimes under different names (such as *bounded real time dynamic programming* [5,23] or *interval iteration* [18]).

BVI comes with a precision guarantee: since $V(\mathcal{G})$ lies between L_i and U_i (whose gap is at most ε), the approximation L_i is at most ε apart from $V(\mathcal{G})$.

The catch, however, is that $\mu\mathbb{X}$ and $\nu\mathbb{X}$ may not coincide, and therefore the overapproximation might not converge to the desired $\mu\mathbb{X}$. This means Algorithm 2 might not terminate. This is the main technical challenge addressed in the previous works on BVI, including [5,20].

In those works, the source of the failure of convergence is identified to be *end components*. See the (very simple) Markov chain in Fig. 1, where the reachability probability from s_I to $\mathbf{1}$ is clearly 0. However, due to the loop between s_I and s, the values $U_i(s_I)$ and $U_i(s)$—these get updated to the average of U_{i-1} at successors—are easily seen to remain 1. Roughly speaking, end components generalize such loops defined in MDPs and SGs (the definitions are graph-theoretic, in terms of strongly connected components). End components cause non-convergence of naive BVI, essentially for the reason we just described.

The solutions previously proposed to this challenge have been to "get rid of end components." For MDPs (1.5 players), the *collapsing* technique detects end components and collapses each of them into a single state [5,18]. After doing so, the Bellman operator $\mathbb{X}$ has a unique fixed point (therefore $\mu\mathbb{X} = \nu\mathbb{X}$), assuring convergence of BVI (Algorithm 2). In the case of SGs (2.5 players), end components cannot simply be collapsed into single states—they must be

handled carefully, taking the "best exits" into account. This is the key idea of the *deflating* technique proposed for SGs in [20].

4 Our Algorithm: Bounded Value Iteration with Upper Bounds Given by Widest Paths

In our algorithm, like in other BVI algorithm, we iteratively construct upper and lower bounds U_i, L_i of the value function $V(\mathcal{G})$ at the same time. See (2). In updating U_i, however, we go beyond the *local* propagation by the Bellman update and conduct *global* propagation, too. This frees us from the curse of end components. The outline of our algorithm is as follows.

- The lower bound L_i is given by $L_i = \mathbb{X}^i \bot$, following Lemma 3.2.2 and Theorem 3.3. This is the same as the other VI algorithms.
- The upper bounds U_i is constructed in the following three steps, using a *global* propagation that takes advantage of fast widest path algorithms.
  - **(Player reduction)** Firstly, we turn the SG $\mathcal{G}$ into an MDP $\mathcal{M}_i$ by fixing Minimizer's strategy to a specific one σ_i.
    Any choice of σ_i would do for the sake of *soundness* (that is, $V(\mathcal{G}) \leq U_i$). However, for *convergence* (that is, $U_i \to V(\mathcal{G})$ as $i \to \infty$), it is important to have $\sigma_0, \sigma_1, \dots$ eventually converge to Minimizer's optimal strategy $\sigma_\bigcirc$. Therefore we let L_i—the current lower estimate of $V(\mathcal{G})$—induce σ_i. Recall that L_i converges to $V(\mathcal{G})$ (Lemma 3.2.2, Theorem 3.3).
  - **(Preprocessing by local propagation)** Secondly, we turn the MDP $\mathcal{M}_i$ into a weighted graph (WG) W_i.
    The construction here is *local* propagation of the previous upper bound U_{i-1}, from each state s to its predecessors in $\mathcal{M}_i$. This is much like an application of the Bellman operator $\mathbb{X}$.
  - **(Global propagation by widest paths)** Finally, we solve the widest path problem in the WG W_i, from each state s to the target state $\mathbf{1}$. The maximum path width from s to $\mathbf{1}$ is used as the value of the upper bound $U_i(s)$.
    This way, we conduct *global* propagation of upper bounds, for which end components pose no threats. Our global propagation is still computationally feasible, thanks to the preprocessing in the previous step that turns a problem on an MDP into one on a WG (modulo some sound approximation).

The use of *global* propagation for upper bounds is a distinguishing feature of our algorithm. This is unlike other BVI algorithms (such as [5,20]) where upper-bound propagation is only local and stepwise. The latter gets trapped when it encounters an EC—therefore some trick such as collapsing [5] and deflating [20] is needed—while our global propagation looks directly at the target state $\mathbf{1}$.

The above outline is presented as pseudocode in Algorithm 3. We describe the three steps in the rest of the section. In particular, we exhibit the definitions of $\mathcal{M}_{\mathrm{PlRd}}$ and $\mathcal{W}_{\mathrm{LcPg}}$ (WPW has been defined and discussed in Definition 2.8), providing some of their properties towards the correctness proof of the algorithm (Sect. 4.3).

Algorithm 3: Our BVI algorithm via widest paths. Here $\mathcal{G} = (S, S_\Box, S_\bigcirc, s_I, \mathbf{1}, \mathbf{0}, A, \mathrm{Av}, \delta)$ is an SG; $\varepsilon > 0$ is a stopping threshold.

```
1 procedure BVI_WP(G, ε)
2     L_0 ← ⊥, U_0 ← ⊤, i ← 0
3     while U_i(s_I) − L_i(s_I) > ε do
4         i++
5         L_i ← 𝕏L_{i−1}                    // value iteration for lower bounds
6         M_i ← M_PlRd(G, L_i)                          // player reduction
7         W_i ← W_LcPg(M_i, U_{i−1})                    // local propagation
8         U_i ← min{U_{i−1}, WPW(W_i)}          // widest path computation
9     return U_i(s_I)
```

4.1 Player Reduction: From SGs to MDPs

The following general definition is not directly used in Algorithm 3. It is used in our theoretical development below, towards the algorithm's correctness.

Definition 4.1 (the MDP $\mathcal{M}(\mathcal{G}, \mathrm{Av}')$). Let $\mathcal{G}$ be the game in Algorithm 3, and $\mathrm{Av}' \colon S \to 2^A$ be such that $\emptyset \neq \mathrm{Av}'(s) \subseteq \mathrm{Av}(s)$ for each $s \in S$.

Then the MDP given by the tuple $(S, S \setminus \{\mathbf{0}\}, \{\mathbf{0}\}, s_I, \mathbf{1}, \mathbf{0}, A, \mathrm{Av}', \delta)$ shall be denoted by $\mathcal{M}(\mathcal{G}, \mathrm{Av}')$, and we say it is induced from $\mathcal{G}$ by restricting Av to Av'.

The above construction consists of 1) restricting actions (from Av to Av'), and 2) turning Minimizer's states into Maximizer's.

The following class of action restrictions will be heavily used.

Definition 4.2 (Minimizer restriction). Let $\mathcal{G}$ be as in Algorithm 3. A *Minimizer restriction* of Av is a function $\mathrm{Av}' \colon S \to 2^A$ such that 1) $\emptyset \neq \mathrm{Av}'(s) \subseteq \mathrm{Av}(s)$ for each $s \in S$, and 2) $\mathrm{Av}'(s) = \mathrm{Av}(s)$ for each state $s \in S_\Box$ of Maximizer's.

In Algorithm 3, we will be using the MDP induced by the following specific Minimizer restriction induced by a function f.

Definition 4.3 (the MDP $\mathcal{M}_{\mathrm{PlRd}}(\mathcal{G}, f)$). Let $\mathcal{G}$ be the game in Algorithm 3, and $f \colon S \to [0,1]$ be a function. The MDP $\mathcal{M}_{\mathrm{PlRd}}(\mathcal{G}, f)$ is defined to be $\mathcal{M}(\mathcal{G}, \mathrm{Av}_f)$ (Definition 4.1), where the function $\mathrm{Av}_f \colon S \to 2^A$ is defined as follows.

$$\begin{aligned} &\mathrm{Av}_f(s) = \mathrm{Av}(s) && \text{for } s \in S_\Box, \\ &\mathrm{Av}_f(s) = \{a \in \mathrm{Av}(s) \mid \forall b \in \mathrm{Av}(s).\, (\mathbb{X}_a f)(s) \leq (\mathbb{X}_b f)(s)\} && \text{for } s \in S_\bigcirc. \end{aligned} \tag{5}$$

The function Av_f is a Minimizer restriction in $\mathcal{G}$ (Definition 4.2).

The intuition of (5) is that $a = \arg\min_{b \in \mathrm{Av}(s)} (\mathbb{X}_b f)(s)$. In the use of this construction in Algorithm 3, the function f will be our "best guess" L_i of the value function $V(\mathcal{G})$. In this situation, $\arg\min_{b \in \mathrm{Av}(s)} (\mathbb{X}_b f)(s)$ is the best action for Minimizer based on the guess $f = L_i$.

Definition 4.4 (the MDP $\mathcal{M}_i$, and Av_i). In Algorithm 3, the MDP $\mathcal{M}_i$ is given by $\mathcal{M}_{\mathrm{PlRd}}(\mathcal{G}, L_i) = \mathcal{M}(\mathcal{G}, \mathrm{Av}_{L_i})$. We write Av_i for available actions in $\mathcal{M}_i$, that is, $\mathcal{M}_i = (S, \mathbf{1}, \mathbf{0}, A, \mathrm{Av}_i, \delta)$.

In the case of Algorithm 3, the MDPs $\mathcal{M}_0, \mathcal{M}_1, \dots$ do not only "converge" to $\mathcal{G}$, but also "reach $\mathcal{G}$ in finitely many steps," in the following sense. The proof is deferred to [24]. The proof relies crucially on the fact that the set $\mathrm{Av}(s)$ of available actions is finite—there is uniform $\varepsilon > 0$ such that every suboptimal action is suboptimal by a gap at least ε.

Lemma 4.5. *In Algorithm 3, there exists $i_{\mathrm{M}} \in \mathbb{N}$ such that, for each $i \geq i_{\mathrm{M}}$, we have $V(\mathcal{G}) = V(\mathcal{M}_i)$.* □

4.2 Local Propagation: From MDPs to WGs

Here is a technical observation that motivates the function $\mathcal{W}_{\mathrm{LcPg}}$.

Lemma 4.6. *Let $\mathcal{G}$ be the game in Algorithm 3, and $\mathrm{Av}' \colon S \to 2^A$ be a Minimizer restriction (Definition 4.2).*

1. *For each state $s \in S$, we have $V(\mathcal{G})(s) \leq \max_{a \in \mathrm{Av}'(s)} \big(\mathbb{X}_a\big(V(\mathcal{G})\big) \big)(s)$.*
2. *For each $k \in \mathbb{N}$, we have*

$$V(\mathcal{G})(s_0) \;\leq \max_{s_0 \xrightarrow{a_0} s_1 \xrightarrow{a_1} \cdots \xrightarrow{a_k} \text{ in } \mathrm{Av}'} \big(\mathbb{X}_{a_k}\big(V(\mathcal{G})\big) \big)(s_k), \tag{6}$$

where the maximum is taken over $a_0, s_1, a_1, \dots, s_k, a_k$ such that $a_0 \in \mathrm{Av}'(s_0), s_1 \in \mathrm{post}(s_0, a_0), a_1 \in \mathrm{Av}'(s_1), \dots, s_k \in \mathrm{post}(s_{k-1}, a_{k-1}), a_k \in \mathrm{Av}'(s_k)$.

Proof. For the item 1, recall that $V(\mathcal{G})$ is the least fixed point of the Bellman operator (Theorem 3.3). For each Minimizer state $s \in S_{\bigcirc}$, we have

$$V(\mathcal{G})(s) = \min_{a \in \mathrm{Av}(s)} \big(\mathbb{X}_a\big(V(\mathcal{G})\big)\big)(s) \leq \min_{a \in \mathrm{Av}'(s)} \big(\mathbb{X}_a\big(V(\mathcal{G})\big)\big)(s) \leq \max_{a \in \mathrm{Av}'(s)} \big(\mathbb{X}_a\big(V(\mathcal{G})\big)\big)(s).$$

For each Maximizer state $s \in S_{\Box}$, we have

$$V(\mathcal{G})(s) = \max_{a \in \mathrm{Av}(s)} \big(\mathbb{X}_a\big(V(\mathcal{G})\big)\big)(s) = \max_{a \in \mathrm{Av}'(s)} \big(\mathbb{X}_a\big(V(\mathcal{G})\big)\big)(s).$$

The latter equality is because Av' does not restrict Maximizer's actions. This proves the item 1.

The item 2 is proved by induction as follows, using the item 1 in its course.

$$
\begin{aligned}
&V(\mathcal{G})(s_0) \\
&\leq \max_{a_0 \in \mathrm{Av}'(s_0)} \big(\mathbb{X}_{a_0}(V(\mathcal{G}))\big)(s_0) \qquad \text{by the item 1.} \\
&= \max_{a_0 \in \mathrm{Av}'(s_0)} \sum_{s_1 \in \mathrm{post}(s_0,a_0)} \delta(s_0,a_0,s_1) \cdot V(\mathcal{G})(s_1) \\
&\leq \max_{a_0 \in \mathrm{Av}'(s_0)} \sum_{s_1 \in \mathrm{post}(s_0,a_0)} \delta(s_0,a_0,s_1) \cdot \Big(\max_{s_1 \xrightarrow{a_1} \cdots \xrightarrow{a_k} \text{ in } \mathrm{Av}'} \big(\mathbb{X}_{a_k}\big(V(\mathcal{G})\big)\big)(s_k) \Big) \\
&\qquad\qquad \text{by the induction hypothesis (for } k-1) \qquad (7) \\
&\leq \max_{a_0 \in \mathrm{Av}'(s_0)} \max_{s_1 \in \mathrm{post}(s_0,a_0)} \Big(\max_{s_1 \xrightarrow{a_1} \cdots \xrightarrow{a_k} \text{ in } \mathrm{Av}'} \big(\mathbb{X}_{a_k}\big(V(\mathcal{G})\big)\big)(s_k) \Big) \\
&= \max_{s_0 \xrightarrow{a_0} s_1 \xrightarrow{a_1} \cdots \xrightarrow{a_k} \text{ in } \mathrm{Av}'} \big(\mathbb{X}_{a_k}\big(V(\mathcal{G})\big)\big)(s_k). \qquad (8)
\end{aligned}
$$

The inequality in (8) holds since an average over s_1 on the left-hand side is replaced by the corresponding maximum on the right-hand side. Note that the value $\max_{s_1 \xrightarrow{a_1} \cdots \xrightarrow{a_k} \text{ in } \mathrm{Av}'} \min_{i \in [1,k]} \big(\mathbb{X}_{a_i}\big(V(\mathcal{G})\big)\big)(s_i)$ that occurs on both sides is determined once s_1 is determined. This concludes the proof. □

Lemma 4.6.2, although not itself used in the following technical development, suggests the idea of global propagation for upper bounds. Note that a bound is given in (6) for each k; it is possible that a bound for some $k > 1$ is tighter than that for $k = 1$, motivating us to take a "look-ahead" further than one step.

However, the bound in (6) is not particularly tuned for tractability: computation of the maximum involves words whose number is exponential in k, and moreover, we want to do so for many k's.

In the end, our main technical contribution is that a similar "look-ahead" can be done by solving the widest path problem in the following weighted graph. The soundness of this method is not so easy as for Lemma 4.6.2—see Sect. 4.3.

Definition 4.7 (the WG $\mathcal{W}_{\mathrm{LcPg}}(\mathcal{M}, f)$). Let $\mathcal{M} = (S, \mathbf{1}, \mathbf{0}, A, \mathrm{Av}', \delta)$ be an MDP, and $f\colon S \to [0,1]$. The WG $\mathcal{W}_{\mathrm{LcPg}}(\mathcal{M}, f)$ is the following triple (S, E, w).

- Its set of vertices is S.
- We have $(s, s') \in E$ if and only if, for some $a \in \mathrm{Av}'(s)$, we have $s' \in \mathrm{post}(s, a)$ (i.e., $\delta(s, a, s') > 0$).
- The weight function $w\colon E \to [0,1]$ is given by

$$
w(s,s') = \max\big\{\, \mathbb{X}_a f(s) \;\big|\; a \in \mathrm{Av}'(s), s' \in \mathrm{post}(s,a) \,\big\}. \qquad (9)
$$

In (9), the function f—that is, the previous upper bound U_{i-1} in Algorithm 3—is propagated one step by the application of $\mathbb{X}_a$. This way of encoding these propagated values as weights in a WG seems pretty rough. For example, in case both s' and s'' are in $\mathrm{post}(s, a)$ for each $a \in \mathrm{Av}'(s)$, we have $w(s, s') = w(s, s'')$, no matter what the transition probabilities from s to s', s'' are. The return

Algorithm 4: A construction of $\mathsf{PATH} : S_{\Diamond \mathbf{1}} \to S^+$ for Lemma 4.8

1 $S_{\mathrm{v}} \leftarrow \{\mathbf{1}\}$, $\mathsf{PATH}(\mathbf{1}) \leftarrow \mathbf{1}$
2 **while** $S_{\Diamond \mathbf{1}} \setminus S_{\mathrm{v}} \neq \emptyset$ **do**
3 Choose a pair of states $(s_{\mathrm{c}}, s_{\mathrm{p}})$ that satisfies the following: $s_{\mathrm{c}} \in S \setminus S_{\mathrm{v}}$, $s_{\mathrm{p}} \in S_{\mathrm{v}}$, $V(\mathcal{G})(s_{\mathrm{c}}) = \max_{s \in S \setminus S_{\mathrm{v}}} V(\mathcal{G})(s)$, and for an optimal action a at s_{c} in $\mathcal{M}$, $s_{\mathrm{p}} \in \mathrm{post}(s_{\mathrm{c}}, a)$
4 $\mathsf{PATH}(s_{\mathrm{c}}) \leftarrow s_{\mathrm{c}} \cdot \mathsf{PATH}(s_{\mathrm{p}})$, $S_{\mathrm{v}} \leftarrow S_{\mathrm{v}} \cup \{s_{\mathrm{c}}\}$
5 **return** PATH

for this paid price (namely the information lost in the rough encoding) is that the resulting data structure (WG) allows fast *global* analysis via the widest path problem. Our experiment results in Sect. 5 demonstrate that this rough yet global approximation can make upper bounds quickly converge.

4.3 Soundness and Convergence

In Algorithm 3, an SG $\mathcal{G}$ is turned into an MDP $\mathcal{M}_i$ and then to a WG $\mathcal{W}_i$. Our claim is that computing a widest path in $\mathcal{W}_i$ gives the next upper bound U_i in the iteration. Here we prove the following correctness properties: soundness ($V(\mathcal{G}) \leq U_i$) and convergence ($U_i \to V(\mathcal{G})$ as $i \to \infty$).

We start with a technical lemma. The choice of the MDP $\mathcal{M}(\mathcal{G}, \mathrm{Av}')$ and the value function $V(\mathcal{G})$ (for $\mathcal{G}$, not for $\mathcal{M}(\mathcal{G}, \mathrm{Av}')$) in the statement is subtle; it turns out to be just what we need.

Lemma 4.8. *Let $\mathcal{G}$ be as in Algorithm 3, and $\mathrm{Av}' \colon S \to 2^A$ be a Minimizer restriction (Definition 4.2). Let $s_0 \in S_{\Diamond \mathbf{1}}$ be a state with a non-zero value (Definition 2.5). Consider the MDP $\mathcal{M}(\mathcal{G}, \mathrm{Av}')$ (Definition 4.1), for which we write simply $\mathcal{M}$. Then there is a finite path $\pi = s_0 a_0 s_1 a_1 \dots a_{n-1} s_n$ in $\mathcal{M}$ that satisfies the following.*

- *The path π reaches $\mathbf{1}$, that is, $s_n = \mathbf{1}$.*
- *Each action is optimal in $\mathcal{M}$ with respect to $V(\mathcal{G})$, that is, $\big(\mathbb{X}_{a_i}\big(V(\mathcal{G})\big)\big)(s_i) = \max_{a \in \mathrm{Av}'(s_i)} \big(\mathbb{X}_a\big(V(\mathcal{G})\big)\big)(s_i)$ for each $i \in [0, n-1]$.*
- *The value function $V(\mathcal{G})$ does not decrease along the path, that is, $V(\mathcal{G})(s_i) \leq V(\mathcal{G})(s_{i+1})$ for each $i \in [0, n-1]$.*

Proof. We construct a function $\mathsf{PATH} : S_{\Diamond \mathbf{1}} \to S^+$ by Algorithm 4. It is clear that PATH assigns a desired path to each $s_0 \in S_{\Diamond \mathbf{1}}$. In particular, $V(\mathcal{G})$ does not decrease along $\mathsf{PATH}(s_0)$ since always a state with a smaller value of $V(\mathcal{G})$ is prepended.

It remains to be shown that, in Line 3, a required pair $(s_{\mathrm{c}}, s_{\mathrm{p}})$ is always found. Let $S_{\mathrm{v}} \subsetneq S_{\Diamond \mathbf{1}}$ be a subset with $\mathbf{1} \in S_{\mathrm{v}}$; here S_{v} is a proper subset of $S_{\Diamond \mathbf{1}}$ since otherwise we should be already out of the while loop (Line 2).

Let $S_{\max} = \{s \in S \setminus S_{\mathrm{v}} \mid V(\mathcal{G})(s) = \max_{s' \in S \setminus S_{\mathrm{v}}} V(\mathcal{G})(s')\}$. Since $S_{\mathrm{v}} \subsetneq S_{\Diamond \mathbf{1}}$, we have $\emptyset \neq S_{\max} \subseteq S_{\Diamond \mathbf{1}}$ and thus $V(\mathcal{G})(s) > 0$ for each $s \in S_{\max}$. We also have $\mathbf{1} \notin S_{\max}$ since $\mathbf{1} \in S_{\mathrm{v}}$.

We argue by contradiction: assume that for any $s \in S \setminus S_{\mathrm{v}}$, $s' \in S_{\mathrm{v}}$, we have $s' \notin \mathrm{post}(s, a_s)$, where a_s is any optimal action at s in $\mathcal{M}$ with respect to $V(\mathcal{G})$.

Now let $s \in S_{\max}$ be an arbitrary element. It follows that $V(\mathcal{G})(s) > 0$.

$$
\begin{aligned}
V(\mathcal{G})(s) &\leq \left(\mathbb{X}_{a_s}(V(\mathcal{G}))\right)(s) \\
&\qquad \text{using Lemma 4.6; here } a_s \text{ is an optimal action at } s \text{ in } \mathcal{M} \text{ with respect to } V(\mathcal{G}), \\
&= \textstyle\sum_{s' \in S \setminus S_{\mathrm{v}}} \delta(s, a_s, s') \cdot V(\mathcal{G})(s') \\
&\qquad\qquad \text{by the assumption that } s' \notin \mathrm{post}(s, a_s) \text{ for each } s' \in S_{\mathrm{v}} \\
&\leq \textstyle\sum_{s' \in S \setminus S_{\mathrm{v}}} \delta(s, a_s, s') \cdot V(\mathcal{G})(s) \\
&\qquad\qquad \text{since } s \in S_{\max} \text{ and hence } V(\mathcal{G})(s') \leq V(\mathcal{G})(s) \\
&= V(\mathcal{G})(s) \qquad \text{since } \textstyle\sum_{s' \in S \setminus S_{\mathrm{v}}} \delta(s_{\mathrm{c}}, a, s') = 1. \qquad (10)
\end{aligned}
$$

Therefore both inequalities in the above must be equalities. In particular, for the second inequality (in (10)) to be an equality, we must have the weight for each suboptimal s' to be 0. That is, $\delta(s, a_s, s') = 0$ for each $s' \in (S \setminus S_{\mathrm{v}}) \setminus S_{\max}$.

The above holds for arbitrary $s \in S_{\max}$. Therefore, for any strategy that is optimal in $\mathcal{M}$ with respect to $V(\mathcal{G})$, once a play is in $S_{\max}$, it never comes out of $S_{\max}$, hence the play never reaches $\mathbf{1}$. Moreover, an optimal strategy in $\mathcal{M}$ with respect to $V(\mathcal{G})$ is at least as good as an optimal strategy for Maximizer in $\mathcal{G}$ (with respect to $V(\mathcal{G})$), that is, the latter reaches $\mathbf{1}$ no more often than the former. This follows from Lemma 4.6. Altogether, we conclude that a Maximizer optimal strategy in $\mathcal{G}$ does not lead any $s \in S_{\max}$ to $\mathbf{1}$, i.e., $V(\mathcal{M})(s) = 0$ for each $s \in S_{\max}$. Now we come to a contradiction. □

In the following lemma, we use the value function $V(\mathcal{G})$ in the position of f in Definition 4.7. This cannot be done in actual execution of Algorithm 4: unlike U_{i-1} in Algorithm 3, the value function $V(\mathcal{G})$ is not known to us. Nevertheless, the lemma is an important theoretical vehicle towards soundness of Algorithm 3.

Lemma 4.9. *Let $\mathcal{G}$ be the game in Algorithm 3, and $\mathrm{Av}' \colon S \to 2^A$ be a Minimizer restriction (Definition 4.2). Let $\mathcal{M} = \mathcal{M}(\mathcal{G}, \mathrm{Av}')$, and $\mathcal{W} = \mathcal{W}_{\mathrm{LcPg}}\big(\mathcal{M}, V(\mathcal{G})\big)$. Then, for each state $s \in S$, we have $\mathrm{WPW}(\mathcal{W})(s, \mathbf{1}) \geq V(\mathcal{G})(s)$.*

Proof. In what follows, we let the WG $\mathcal{W} = \mathcal{W}_{\mathrm{LcPg}}\big(\mathcal{M}, V(\mathcal{G})\big)$ be denoted by $\mathcal{W} = (S, E, w)$. Let $\pi = s_0 a_0 s_1 a_1 \dots a_{n-1} s_n$ be a path of the MDP $\mathcal{M}$ such that $s_n = \mathbf{1}$, each action is optimal in $\mathcal{M}$ with respect to $V(\mathcal{G})$, and $V(\mathcal{G})(s_i) \leq V(\mathcal{G})(s_{i+1})$ for each $i \in [0, n-1]$. Existence of such a path π is shown by Lemma 4.8. Let $\pi' = s_0 s_1 \dots s_{n-1} \mathbf{1}$ be the path in the WG $\mathcal{W}$ induced by π—we simply omit actions.

The path π' satisfies the following, for each $i \in [0, n-1]$.

$$
\begin{aligned}
w(s_i, s_{i+1}) &= \max\{\, (\mathbb{X}_a(V(\mathcal{G})))(s_i) \mid a \in \mathrm{Av}'(s_i), s_{i+1} \in \mathrm{post}(s_i, a) \,\} \quad \text{by Definition 4.7} \\
&= (\mathbb{X}_{a_i}(V(\mathcal{G})))(s_i) \quad \text{since } a_i \text{ is optimal wrt. } V(\mathcal{G}); \\
&\quad \text{note that } a_i \in \mathrm{Av}'(s_i), s_{i+1} \in \mathrm{post}(s_i, a_i) \text{ hold since } \pi \text{ is a path in } \mathcal{M} \\
&= \max_{a \in \mathrm{Av}'(s)} (\mathbb{X}_a(V(\mathcal{G})))(s_i) \quad \text{since } a_i \text{ is optimal wrt. } V(\mathcal{G}) \\
&\geq V(\mathcal{G})(s_i) \qquad \text{by Lemma 4.6.}
\end{aligned}
$$

This observation, combined with $V(\mathcal{G})(s_0) \leq V(\mathcal{G})(s_1) \leq \cdots \leq V(\mathcal{G})(s_n)$ (by the definition of π), implies that the width of the path π' is at least $V(\mathcal{G})(s_0)$. The widest path width is no smaller than that. □

Theorem 4.10 (soundness). *In Algorithm 3, $V(\mathcal{G}) \leq U_i$ holds for each $i \in \mathbb{N}$.*

Proof. We let the function

$$
\begin{aligned}
&\min\{\, U,\ \mathrm{WPW}(\mathcal{W}_{\mathrm{LcPg}}(\mathcal{M}(\mathcal{G}, \mathrm{Av}'), U))(\_, \mathbf{1}) \,\} \quad : \quad S \longrightarrow [0,1] \\
&\text{denoted by} \qquad T(\mathrm{Av}', U) : \quad S \longrightarrow [0,1],
\end{aligned}
$$

clarifying its dependence on Av' and $U \colon S \to [0,1]$. Clearly, for each $i \in \mathbb{N}$, we have $U_i = T(\mathrm{Av}_{L_i}, U_{i-1})$.

The rest of the proof is by induction. It is trivial if $i = 0$ ($U_0 = \top$).

$$
\begin{aligned}
U_{i+1} &= T(\mathrm{Av}_{L_i}, U_i) \\
&\geq T(\mathrm{Av}_{L_i}, V(\mathcal{G})) \qquad \text{by ind. hyp., and } T(\mathrm{Av}_{L_i}, \_) \text{ is monotone} \\
&= \min\{\, V(\mathcal{G}),\ \mathrm{WPW}(\mathcal{W}_{\mathrm{LcPg}}(\mathcal{M}(\mathcal{G}, \mathrm{Av}_{L_i}), V(\mathcal{G})))(\_, \mathbf{1}) \,\} \\
&= V(\mathcal{G}) \qquad \text{by Lemma 4.9.}
\end{aligned}
$$

□

It is clear that U_i decreases with respect to i ($U_0 \geq U_1 \geq \cdots$), by the presence of min in Line 8. It remains to show the following.

Theorem 4.11 (convergence). *In Algorithm 3, let the while loop iterate forever. Then $U_i \to V(\mathcal{G})$ as $i \to \infty$.*

Proof. We give a proof using the infinitary pigeonhole principle. The proof is nonconstructive—it is not suited for analyzing the speed of convergence, for example—but the proof becomes simpler.

In what follows, we let $\mathbb{X}_\sigma \colon (S \to [0,1]) \to (S \to [0,1])$ denote the Bellman operator on an MDP $\mathcal{M}$ induced by a strategy σ, i.e., $(\mathbb{X}_\sigma f)(s) := (\mathbb{X}_{\sigma(s)} f)(s)$. The MC obtained from an MDP $\mathcal{M}$ by fixing a strategy σ is denoted by $\mathcal{M}^\sigma$.

Towards the statement of the theorem, for each $i \in \mathbb{N}$, we choose a (positional) strategy σ_i in the MDP $\mathcal{M}_i$ as follows.

– For each $s \in S_{\Diamond\mathbf{1}}$, take the widest path $\mathrm{WPath}(\mathcal{W}_i, \mathbf{1})(s) = ss_1 \dots \mathbf{1}$ in $\mathcal{W}_i$ from s to $\mathbf{1}$ (Definition 2.8). Such a path from s to $\mathbf{1}$ exists—otherwise we have $U_i(s) = 0$, hence $V(\mathcal{G})(s) = 0$ by Theorem 4.10.
Let $\sigma_i(s)$ be an action that justifies the first edge in the chosen widest path, that is, $a \in \mathrm{Av}_i(s)$ such that $s_1 \in \mathrm{post}(s, a)$.
– For each $s \in S \setminus S_{\Diamond\mathbf{1}}$, $\sigma_i(s)$ is freely chosen from $\mathrm{Av}_i(s)$.

It is then easy to see that

$$\mathrm{WPW}(\mathcal{W}_i)(s) \le (\mathbb{X}_{\sigma_i} U_{i-1})(s) \qquad \text{for each } i \in \mathbb{N} \text{ and } s \in S_{\Diamond\mathbf{1}}. \tag{11}$$

Indeed, by the definition of σ_i, the right-hand side is the weight of the first edge in the chosen widest path. This must be no smaller than the widest path width, that is, the width of the chosen path.

Now, since there are only finitely many strategies for the SG $\mathcal{G}$, the same is true for the MDPs $\mathcal{M}_0, \mathcal{M}_1, \dots$ that are obtained from $\mathcal{G}$ by restricting Minimizer's actions. Therefore, by the infinitary pigeonhole principle, there are infinitely many $i_0 < i_1 < \cdots$ such that $\sigma_{i_0} = \sigma_{i_1} = \cdots \quad =: \sigma^\dagger$. Moreover, we can choose them so that they are all beyond i_{M} in Lemma 4.5, in which case we have

$$V(\mathcal{M}_{i_m}^{\sigma^\dagger}) \le V(\mathcal{G}) \quad \text{for each } m \in \mathbb{N}. \tag{12}$$

Indeed, Minimizer's actions are already optimized in $\mathcal{M}_i$ (Lemma 4.5), and thus the only freedom left for $\sigma^\dagger$ is to choose suboptimal actions of Maximizer's.

In what follows, we cut down the domain of discourse from $S \to [0,1]$ to $S_{\Diamond\mathbf{1}} \to [0,1]$, i.e., 1) every function of the type $f : S \to [0,1]$ is now seen as the restriction over $S_{\Diamond\mathbf{1}}$, and 2) the Bellman operator only adds up the value of the input function over $S_{\Diamond\mathbf{1}}$, namely it is now defined by $\hat{\mathbb{X}}_a f(s) = \sum_{s' \in S_{\Diamond\mathbf{1}}} \delta(s, a, s') \cdot f(s')$. The operator $\hat{\mathbb{X}}_\sigma$ is also defined in a similar way to $\mathbb{X}_\sigma$.

Now proving convergence in $S_{\Diamond\mathbf{1}} \to [0,1]$ suffices for the theorem. Indeed, for each $i \ge i_{\mathrm{M}}$, we have $V(\mathcal{M}_i)(s) = V(\mathcal{G})(s) = 0$ for each $s \in S \setminus S_{\Diamond\mathbf{1}}$. This implies that there is no path from s to $\mathbf{1}$ in $\mathcal{M}_i$, thus neither in the WG $\mathcal{W}_i$. Therefore $U_i \le \mathrm{WPW}(\mathcal{W}_i) = 0$.

A benefit of this domain restriction is that the Bellman operator $\hat{\mathbb{X}}_\sigma$ has a unique fixed point in $S_{\Diamond\mathbf{1}} \to [0,1]$ if the set of non-sink states in $\mathcal{M}^\sigma$ is exactly $S_{\Diamond\mathbf{1}}$, i.e., $V(\mathcal{M}^\sigma)(s) > 0$ holds if and only if $s \in S_{\Diamond\mathbf{1}}$. Furthermore, this unique fixed point is the value function $V(\mathcal{M}^\sigma)$ restricted to $S_{\Diamond\mathbf{1}} \subseteq S$ [4, Theorem 10.19]. Therefore $V(\mathcal{M}^\sigma)$ is computed by the gfp Kleene iteration, too:

$$\top \ge \hat{\mathbb{X}}_\sigma \top \ge (\hat{\mathbb{X}}_\sigma)^2 \top \ge \cdots \longrightarrow V(\mathcal{M}^\sigma) \quad \text{in the space } S_{\Diamond\mathbf{1}} \to [0,1]. \tag{13}$$

We show the following by induction on m.

$$U_{i_m} \le (\hat{\mathbb{X}}_{\sigma^\dagger})^m \top \quad \text{for each } m \in \mathbb{N}. \tag{14}$$

It is obvious for $m = 0$. For the step case, we have the following. Notice that the inequality (11) holds in the restricted domain for $i \geq i_M$.

$$\begin{aligned} U_{i_{m+1}} &\leq \mathrm{WPW}(\mathcal{W}_{i_{m+1}}) \quad \text{by Line 8 of Algorithm 3} \\ &\leq \hat{\mathbb{X}}_{\sigma^\dagger} U_{i_{m+1}-1} \quad \text{by (11)} \\ &\leq \hat{\mathbb{X}}_{\sigma^\dagger} U_{i_m} \quad \text{by monotonicity of } \hat{\mathbb{X}}_{\sigma^\dagger}, \text{ decrease of } U_i \text{ and } i_m < i_{m+1} \\ &\leq (\hat{\mathbb{X}}_{\sigma^\dagger})^{m+1} \top \quad \text{by the induction hypothesis.} \end{aligned}$$

We have proved (14) which proves $\inf_i U_i \leq \inf_m (\hat{\mathbb{X}}_{\sigma^\dagger})^m \top$.

Lastly, we prove that $V(\mathcal{M}_{i_m}^{\sigma^\dagger})(s) > 0$ holds if and only if $s \in S_{\Diamond \mathbf{1}}$ for each $m \in \mathbb{N}$, and thus $\sigma^\dagger$ follows the characterization in (13). This proves

$$\inf_i U_i \leq V(\mathcal{M}_{i_m}^{\sigma^\dagger}) \quad \text{for each } m \in \mathbb{N}. \tag{15}$$

Implication to the right is clear as Minimizer restriction is done optimally in $\mathcal{M}_{i_m}$. Conversely, if $s \in S_{\Diamond \mathbf{1}}$, then there is a path from s to $\mathbf{1}$ in $\mathcal{W}_{i_m}$. Let $\mathrm{WPath}(\mathcal{W}_{i_m}, \mathbf{1})(s) = s_0 s_1 \dots s_k$, where $s_0 = s$, $k \in \mathbb{N}$ and $s_k = \mathbf{1}$. Then by the property of WPath and $\sigma^\dagger$, we have $\delta(s_j, \sigma^\dagger(s_j), s_{j+1}) > 0$ for each $j < k$. Thus, the probability that the finite path $\mathrm{WPath}(\mathcal{W}_{i_m}, \mathbf{1})(s)$ is obtained by running $\mathcal{M}_{i_m}^{\sigma^\dagger}$ starting from s, which is apparently at most $V(\mathcal{M}_{i_m}^{\sigma^\dagger})(s)$, is nonzero. Hence we have implication to the left.

Combining (12), (15) and Theorem 4.10, we obtain the claim. □

5 Experiment Results

Experiment Settings. We compare the following four algorithms.

- *WP* is our BVI algorithm via widest paths. It avoids end component (EC) computation by global propagation of upper bounds.
- *DFL* is the implementation of the main algorithm in [20]. It relies on EC computation for deflating.
- *DFL_m* is our modification of DFL, where some unnecessary repetition of EC computation is removed.
- *DFL_BRTDP* is the learning-based variant of DFL. It restricts bound update to those states which are visited by simulations. See [20] for details.

The latter three—coming from [20]—are the only existing BVI algorithms for SGs with a convergence guarantee, to the best of our knowledge. The implementation of DFL and DFL_BRTDP is provided by the authors of [20].

The four algorithms are implemented on top of PRISM-games [21] version 2.0. We used the stopping threshold $\varepsilon = 10^{-6}$. The experiments were conducted on Dell Inspiron 3421 Laptop with 4.00 GB RAM and Intel(R) Core(TM) i5-3337U 1.80 GHz processor.

In the implementations of DFL and DFL_BRTDP, the deflating operation is applied only once every five iterations [20, Sect. B.3]. Following this, our WP also

solves the widest path problem (Line 8) only once every five iterations, while other operations are applied in each iteration.

For input SGs, we took four models from the literature: *mdsm* [11], *cloud* [6], *teamform* [12] and *investor* [22]. In addition, we used our model *manyECs*—an artificial model with many ECs—to assess the effect of ECs on performance. The model manyECs is presented in the appendix in [24]. Each of these five models comes with a model parameter N.

There is another model called *cdmsn* in [20]. We do not discuss cdmsn since all the algorithms (ours and those from [20]) terminated within 0.001 seconds.

Results. The number i of iterations and the running time for each algorithm and each input SG is shown in Table 1. For DFL_BRTDP, the ratio of states visited by the algorithm is shown in percentage; the smaller it is, the more efficient the algorithm is in reducing the state space. Each number for DFL_BRTDP (a probabilistic algorithm) is the average over 5 runs.

Table 1. Experimental results, comparing WP (our algorithm) with those in [20]. N is a model parameter (the bigger the more complex). #states, #trans, #EC show the numbers of states, transitions and ECs in the SG, respectively. itr is the number i of iterations at termination; time is the execution time in seconds. For each SG, the fastest algorithm is shaded in green. The settings that did not terminate are shaded in gray; TO is time out (6 h), OOM is out of memory, and SO is stack overflow.

model	N	#states	#trans	#EC	DFL		DFL_m		DFL_BRTDP			WP	
					itr	time	itr	time	itr	visit%	time	itr	time
mdsm	3	62245	151143	1	121	3	121	4	17339	49.3	15	120	5
	4	335211	882765	1	125	15	125	47	91301	42.1	86	124	38
cloud	5	8842	60437	4421	7	7	7	1	167	6.9	14	7	<1
	6	34954	274965	17477	11	177	11	5	41	0.6	3	11	1
	7	139402	1237525	69701	11	19721	11	62	41	0.2	4	11	5
teamform	3	12475	15228	2754	2	<1	2	<1	972	49.0	137	2	<1
	4	96665	116464	19800	2	<1	2	<1	4154	34.6	9603	2	<1
	5	907993	1084752	176760	2	<1	2	<1			TO	2	<1
investor	50	211321	673810	29690	441	184	441	249			TO	364	48
	100	807521	2587510	114390	801	3318		OOM			TO	688	736
manyECs	500	1004	3007	502	6	7	6	7			TO	5	<1
	1000	2004	6007	1002	6	51	6	51			TO	5	<1
	5000	10004	30007	5002		SO		SO			TO	5	<1

Discussion. We observe consistent performance advantage of our algorithm (WP). Even in the mdsm model where the DFL algorithms do not suffer from EC computation (#EC is just 1), WP's performance is comparable to DFL. The cloud model is where the learning-based approach in [20] works well—see visit% that are very small. Our WP performs comparably against DFL_BRTDP, too.

The performance advantage of our WP algorithm is eminent, not only in the artificial model of manyECs (where WP is faster by magnitudes), but also in

the realistic model investor that comes from a financial application scenario [22]. The results for these two models suggest that WP is indeed advantageous when EC computation poses a bottleneck for other algorithms.

Overall, we observe that our WP algorithm can be the first choice when it comes to solving SGs: for some models, it runs much faster than other algorithms; for other models, even if the performances of other algorithms differs a lot, WP's performance is comparable with the best algorithm.

6 Conclusions and Future Work

In this paper, we presented a new BVI algorithm for solving stochastic games. It features global propagation of upper bounds by widest paths, via a novel encoding of the problem to a suitable weighted graph. This way we avoid computation of end components that often penalizes the performance of the other BVI-based algorithms. Our experimental comparison with known BVI algorithms for SGs demonstrates the efficiency of our algorithm. For correctness of the algorithm, we presented proofs for soundness and convergence.

Extending the current algorithm for more advanced settings is future work—this is much like the results in [20] are extended and used in [2,3,16]. In doing so, we hope to make essential use of structures that are unique to those advanced problem settings. Another important direction is to push forward the idea of global propagation in verification and synthesis, seeking further instances of the idea. Finally, pursuing the global propagation idea in the context of reinforcement learning—where problems are often formalized using MDPs and the Bellman operator is heavily utilized—may open up another fruitful collaboration between formal methods and statistical machine learning.

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