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New York City, NY, USA, July 15–18, 2019
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Preface

It was our privilege to serve as the program chairs for CAV 2019, the 31st International Conference on Computer-Aided Verification. CAV 2019 was held in New York, USA, during July 15–18, 2019. The tutorial day was on July 14, 2019, and the pre-conference workshops were held during July 13–14, 2019. All events took place in The New School in New York City.

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 put CAV at the cutting edge of formal methods research, and this year's program is a reflection of this commitment.

CAV 2019 received a very high number of submissions (258). We accepted 13 tool papers, two case studies, and 52 regular papers, which amounts to an acceptance rate of roughly 26%. 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, learning, and industrially deployed systems. The program featured invited talks by Dawn Song (UC Berkeley), Swarat Chaudhuri (Rice University), and Ken McMillan (Microsoft Research) as well as invited tutorials by Emina Torlak (University of Washington) and Ranjit Jhala (UC San Diego). 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 2019 hosted the following workshops: The Best of Model Checking (BeMC) in honor of Orna Grumberg, Design and Analysis of Robust Systems (DARS), Verification Mentoring Workshop (VMW), Numerical Software Verification (NSV), Verified Software: Theories, Tools, and Experiments (VSTTE), Democratizing Software Verification, Formal Methods for ML-Enabled Autonomous Systems (FoMLAS), and Synthesis (SYNT).

Organizing a top conference like CAV requires a great deal of effort from the community. The Program Committee for CAV 2019 consisted of 79 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 770 reviews while investing significant effort to maintain and ensure the high quality of the conference program. We are grateful to the CAV 2019 Program Committee 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 artifact evaluation mandatory for tool submissions and optional but encouraged for the rest of the accepted papers. The Artifact Evaluation Committee consisted of 27 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 regular papers, 65% 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.

CAV 2019 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 2019 a success. First, we would like to thank Yu Feng and Ruben Martins for chairing the Artifact Evaluation Committee and Zvonimir Rakamaric for maintaining the CAV website and social media presence. We also thank Oksana Tkachuk for chairing the workshop organization process, Peter O'Hearn for managing sponsorship, and Thomas Wies for arranging student fellowships. We also thank Loris D'Antoni, Rayna Dimitrova, Cezara Dragoi, and Anthony W. Lin for organizing the Verification Mentoring Workshop and working closely with us. Last but not least, we would like to thank Kostas Ferles, Navid Yaghmazadeh, and members of the CAV Steering Committee (Ken McMillan, Aarti Gupta, Orna Grumberg, and Daniel Kroening) for helping us with several important aspects of organizing CAV 2019.

We hope that you will find the proceedings of CAV 2019 scientifically interesting and thought-provoking!

June 2019

Isil Dillig
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Symbolic Register Automata

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Abstract. Symbolic Finite Automata and Register Automata are two orthogonal extensions of finite automata motivated by real-world problems where data may have unbounded domains. These automata address a demand for a model over large or infinite alphabets, respectively. Both automata models have interesting applications and have been successful in their own right. In this paper, we introduce Symbolic Register Automata, a new model that combines features from both symbolic and register automata, with a view on applications that were previously out of reach. We study their properties and provide algorithms for emptiness, inclusion and equivalence checking, together with experimental results.

1 Introduction

Finite automata are a ubiquitous formalism that is simple enough to model many real-life systems and phenomena. They enjoy a large variety of theoretical properties that in turn play a role in practical applications. For example, finite automata are closed under Boolean operations, and have decidable emptiness and equivalence checking procedures. Unfortunately, finite automata have a fundamental limitation: they can only operate over finite (and typically small) alphabets. Two *orthogonal* families of automata models have been proposed to overcome this: *symbolic automata* and *register automata*. In this paper, we show that these two models can be combined yielding a new powerful model that can cover interesting applications previously out of reach for existing models.

Symbolic finite automata (SFAs) allow transitions to carry predicates over rich first-order alphabet theories, such as linear arithmetic, and therefore extend classic automata to operate over infinite alphabets [12]. For example, an SFA can define the language of all lists of integers in which the first and last elements are positive integer numbers. Despite their increased expressiveness, SFAs enjoy the same closure and decidability properties of finite automata—e.g., closure under Boolean operations and decidable equivalence and emptiness.

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Register automata (RA) support infinite alphabets by allowing input characters to be stored in registers during the computation and to be compared against existing values that are already stored in the registers [17]. For example, an RA can define the language of all lists of integers in which all numbers appearing in even positions are the same. RAs do not have some of the properties of finite automata (e.g., they cannot be determinized), but they still enjoy many useful properties that have made them a popular model in static analysis, software verification, and program monitoring [15].

In this paper, we combine the best features of these two models—first order alphabet theories and registers—into a new model, *symbolic register automata* (SRA). SRAs are strictly more expressive than SFAs and RAs. For example, an SRA can define the language of all lists of integers in which the first and last elements are positive rational numbers and all numbers appearing in even positions are the same. This language is not recognizable by either an SFA nor by an RA.

While other attempts at combining symbolic automata and registers have resulted in undecidable models with limited closure properties [11], we show that SRAs enjoy the same closure and decidability properties of (non-symbolic) register automata. We propose a new application enabled by SRAs and implement our model in an open-source automata library.

In summary, our contributions are:

- Symbolic Register Automata (SRA): a new automaton model that can handle complex alphabet theories while allowing symbols at arbitrary positions in the input string to be compared using equality (Sect. 3).
- A thorough study of the properties of SRAs. We show that SRAs are closed under intersection, union and (deterministic) complementation, and provide algorithms for emptiness and forward (bi)simulation (Sect. 4).
- A study of the effectiveness of our SRA implementation on handling regular expressions with back-references (Sect. 5). We compile a set of benchmarks from existing regular expressions with back-references (e.g., `(\d)[a-z]*\1`) and show that SRAs are an effective model for such expressions and existing models such as SFAs and RAs are not. Moreover, we show that SRAs are more efficient than the `java.util.regex` library for matching regular expressions with back-references.

2 Motivating Example

In this section, we illustrate the capabilities of symbolic register automata using a simple example. Consider the regular expression r_p shown in Fig. 1a. This expression, given a sequence of product descriptions, checks whether the products have the same code and lot number. The reader might not be familiar with some of the unusual syntax of this expression. In particular, r_p uses two back-references `\1` and `\2`. The semantics of this construct is that the string matched by the regular expression for `\1` (resp. `\2`) should be exactly the string that matched the subregular expression r appearing between the first (resp. second)

```
C:(.{3}) L:(.) D:[^\s]+( C:\1 L:\2 D:[^\s]+)+
```

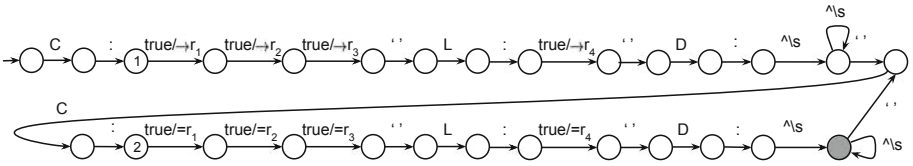
(a) Regular expression r_p (with back-reference).

```
C:X4a L:4 D:bottle C:X4a L:4 D:jar
```

(b) Example text matched by r_p.

```
C:X4a L:4 D:bottle C:X5a L:4 D:jar
```

(c) Example text *not* matched by r_p.



(d) Snippets of a symbolic register automaton A_p corresponding to r_p.

Fig. 1. Regular expression for matching products with same code and lot number—i.e., the characters of C and L are the same in all the products.

two parenthesis, in this case `(.{3})` (resp. `(.)`). Back-references allow regular expressions to check whether the encountered text is the same or is different from a string/character that appeared earlier in the input (see Figs. 1b and c for examples of positive and negative matches).

Representing this complex regular expression using an automaton model requires addressing several challenges. The expression r_p:

1. operates over large input alphabets consisting of upwards of 2^{16} characters;
2. uses complex character classes (e.g., `\s`) to describe different sets of characters in the input;
3. adopts back-references to detect repeated strings in the input.

Existing automata models do not address one or more of these challenges. Finite automata require one transition for each character in the input alphabet and blow-up when representing large alphabets. Symbolic finite automata (SFA) allow transitions to carry predicates over rich structured first-order alphabet theories and can describe, for example, character classes [12]. However, SFAs cannot directly check whether a character or a string is repeated in the input. An SFA for describing the regular expression r_p would have to store the characters after `C:` directly in the states to later check whether they match the ones of the second product. Hence, the smallest SFA for this example would require billions of states! Register automata (RA) and their variants can store characters in registers during the computation and compare characters against values already stored in the registers [17]. Hence, RAs can check whether the two products have the same code. However, RAs only operate over unstructured infinite alphabets and cannot check, for example, that a character belongs to a given class.

The model we propose in this paper, *symbolic register automata* (SRA), combines the best features of SFAs and RAs—first-order alphabet theories and registers—and can address all the three aforementioned challenges. Figure 1d shows a snippet of a symbolic register automaton A_p corresponding to r_p. Each transition in A_p is labeled with a predicate that describes what characters can

trigger the transition. For example, `^\s` denotes that the transition can be triggered by any non-space character, `L` denotes that the transition can be triggered by the character `L`, and `true` denotes that the transition can be triggered by any character. Transitions of the form $\varphi/\rightarrow r_i$ denote that, if a character x satisfies the predicate φ, the character is then stored in the register r_i. For example, the transition out of state 1 reads any character and stores it in register r_1. Finally, transitions of the form $\varphi/= r_i$ are triggered if a character x satisfies the predicate φ and x is the same character as the one stored in r_i. For example, the transition out of state 2 can only be triggered by the same character that was stored in r_1 when reading the transition out state 1—i.e., the first characters in the product codes should be the same.

SRAs are a natural model for describing regular expressions like r_p, where capture groups are of bounded length, and hence correspond to finitely-many registers. The SRA A_p has fewer than 50 states (vs. more than 100 billion for SFAs) and can, for example, be used to check whether an input string matches the given regular expression (e.g., monitoring). More interestingly, in this paper we study the closure and decidability properties of SRAs and provide an implementation for our model. For example, consider the following regular expression r_{pC} that only checks whether the product codes are the same, but not the lot numbers:

```
C:(.{3}) L:. D:[^\s]+( C:\1 L:. D:[^\s]+)+
```

The set of strings accepted by r_{pC} is a superset of the set of strings accepted by r_p. In this paper, we present simulation and bisimulation algorithms that can check this property. Our implementation can show that r_p subsumes r_{pC} in 25 s and we could not find other tools that can prove the same property.

3 Symbolic Register Automata

In this section we introduce some preliminary notions, we define symbolic register automata and a variant that will be useful in proving decidability properties.

Preliminaries. An *effective Boolean algebra* $\mathcal{A}$ is a tuple $(\mathcal{D}, \Psi, [\![\_]\!], \bot, \top, \wedge, \vee, \neg)$, where: $\mathcal{D}$ is a set of domain elements; Ψ is a set of predicates closed under the Boolean connectives and $\bot, \top \in \Psi$. The denotation function $[\![\_]\!]\colon \Psi \to 2^{\mathcal{D}}$ is such that $[\![\bot]\!] = \emptyset$ and $[\![\top]\!] = \mathcal{D}$, for all $\varphi, \psi \in \Psi$, $[\![\varphi \vee \psi]\!] = [\![\varphi]\!] \cup [\![\psi]\!]$, $[\![\varphi \wedge \psi]\!] = [\![\varphi]\!] \cap [\![\psi]\!]$, and $[\![\neg\varphi]\!] = \mathcal{D} \setminus [\![\varphi]\!]$. For $\varphi \in \Psi$, we write $\mathsf{isSat}(\varphi)$ whenever $[\![\varphi]\!] \neq \emptyset$ and say that φ is *satisfiable*. $\mathcal{A}$ is *decidable* if isSat is decidable. For each $a \in \mathcal{D}$, we assume predicates $\mathsf{atom}(a)$ such that $[\![\mathsf{atom}(a)]\!] = \{a\}$.

Example 1. The theory of linear integer arithmetic forms an effective BA, where $\mathcal{D} = \mathbb{Z}$ and Ψ contains formulas $\varphi(x)$ in the theory with one fixed integer variable. For example, $\mathsf{div_k} \coloneqq (x \bmod k) = 0$ denotes the set of all integers divisible by k.

Notation. Given a set S, we write $\mathcal{P}(S)$ for its powerset. Given a function $f\colon A \to B$, we write $f[a \mapsto b]$ for the function such that $f[a \mapsto b](a) = b$ and $f[a \mapsto b](x) = f(x)$, for $x \neq a$. Analogously, we write $f[S \mapsto b]$, with $S \subseteq A$, to map multiple values to the same b. The *pre-image* of f is the function $f^{-1}\colon \mathcal{P}(B) \to \mathcal{P}(A)$ given by $f^{-1}(S) = \{a \mid \exists b \in S\colon b = f(a)\}$; for readability, we will write $f^{-1}(x)$ when $S = \{x\}$. Given a relation $\mathcal{R} \subseteq A \times B$, we write $a\mathcal{R}b$ for $(a, b) \in \mathcal{R}$.

Model Definition. Symbolic register automata have transitions of the form:

$$p \xrightarrow{\varphi/E,I,U} q$$

where p and q are states, φ is a predicate from a fixed effective Boolean algebra, and E, I, U are subsets of a fixed finite set of registers R. The intended interpretation of the above transition is: an input character a can be read in state q if (i) $a \in [\![\varphi]\!]$, (ii) the content of all the registers in E is *equal* to a, and (iii) the content of all the registers in I is *different* from a. If the transition succeeds then a is stored into all the registers U and the automaton moves to q.

Example 2. The transition labels in Fig. 1d have been conveniently simplified to ease intuition. These labels correspond to full SRA labels as follows:

$$\varphi/{\to}r \implies \varphi/\emptyset,\emptyset,\{r\} \qquad \varphi/{=}r \implies \varphi/\{r\},\emptyset,\emptyset \qquad \varphi \implies \varphi/\emptyset,\emptyset,\emptyset\ .$$

Given a set of registers R, the transitions of an SRA have labels over the following set: $L_R = \Psi \times \{(E, I, U) \in \mathcal{P}(R) \times \mathcal{P}(R) \times \mathcal{P}(R) \mid E \cap I = \emptyset\}$. The condition $E \cap I = \emptyset$ guarantees that register constraints are always satisfiable.

Definition 1 (Symbolic Register Automaton). *A* symbolic register automaton *(SRA) is a 6-tuple $(R, Q, q_0, v_0, F, \Delta)$, where R is a finite set of* registers*, Q is a finite set of* states*, $q_0 \in Q$ is the* initial *state, $v_0\colon R \to \mathcal{D} \cup \{\sharp\}$ is the* initial register assignment *(if $v_0(r) = \sharp$, the register r is considered* empty*), $F \subseteq Q$ is a finite set of* final *states, and $\Delta \subseteq Q \times L_R \times Q$ is the* transition relation*. Transitions $(p, (\varphi, \ell), q) \in \Delta$ will be written as $p \xrightarrow{\varphi/\ell} q$.*

An SRA can be seen as a finite description of a (possibly infinite) labeled transition system (LTS), where states have been assigned concrete register values, and transitions read a single symbol from the potentially infinite alphabet. This so-called *configuration LTS* will be used in defining the semantics of SRAs.

Definition 2 (Configuration LTS). *Given an SRA $\mathcal{S}$, the* configuration *LTS* $\mathsf{CLTS}(\mathcal{S})$ *is defined as follows. A* configuration *is a pair (p, v) where $p \in Q$ is a state in $\mathcal{S}$ and a $v\colon R \to \mathcal{D} \cup \{\sharp\}$ is* register assignment*; (q_0, v_0) is called the* initial configuration*; every (q, v) such that $q \in F$ is a* final *configuration. The set of transitions between configurations is defined as follows:*

$$\frac{p \xrightarrow{\varphi/E,I,U} q \in \Delta \qquad E \subseteq v^{-1}(a) \quad I \cap v^{-1}(a) = \emptyset}{(p, v) \xrightarrow{a} (q, v[U \mapsto a]) \in \mathsf{CLTS}(\mathcal{S})}$$

Intuitively, the rule says that a SRA transition from p can be instantiated to one from (p, v) that reads a when the registers containing the value a, namely $v^{-1}(a)$, satisfy the constraint described by E, I (a is contained in registers E but not in I). If the constraint is satisfied, all registers in U are assigned a.

A *run* of the SRA $\mathcal{S}$ is a sequence of transitions in $\mathsf{CLTS}(\mathcal{S})$ starting from the initial configuration. A configuration is *reachable* whenever there is a run ending up in that configuration. The *language* of an SRA $\mathcal{S}$ is defined as

$$\mathscr{L}(\mathcal{S}) := \{a_1 \dots a_n \in \mathcal{D}^n \mid \exists (q_0, v_0) \xrightarrow{a_1} \dots \xrightarrow{a_n} (q_n, v_n) \in \mathsf{CLTS}(\mathcal{S}), q_n \in F\}$$

An SRA $\mathcal{S}$ is *deterministic* if its configuration LTS is; namely, for every word $w \in \mathcal{D}^\star$ there is at most one run in $\mathsf{CLTS}(\mathcal{S})$ spelling w. Determinism is important for some application contexts, e.g., for runtime monitoring. Since SRAs subsume RAs, nondeterministic SRAs are strictly more expressive than deterministic ones, and language equivalence is undecidable for nondeterministic SRAs [27].

We now introduce the notions of *simulation* and *bisimulation* for SRAs, which capture whether one SRA behaves "at least as" or "exactly as" another one.

Definition 3 ((Bi)simulation for SRAs). *A simulation $\mathcal{R}$ on SRAs $\mathcal{S}_1$ and $\mathcal{S}_2$ is a binary relation $\mathcal{R}$ on configurations such that $(p_1, v_1)\mathcal{R}(p_2, v_2)$ implies:*

- *if $p_1 \in F_1$ then $p_2 \in F_2$;*
- *for each transition $(p_1, v_1) \xrightarrow{a} (q_1, w_1)$ in $\mathsf{CLTS}(\mathcal{S}_1)$, there exists a transition $(p_2, v_2) \xrightarrow{a} (q_2, w_2)$ in $\mathsf{CLTS}(\mathcal{S}_2)$ such that $(q_1, w_1)\mathcal{R}(q_2, w_2)$.*

A simulation $\mathcal{R}$ is a bisimulation *if $\mathcal{R}^{-1}$ is a also a simulation. We write $\mathcal{S}_1 \prec \mathcal{S}_2$ (resp. $\mathcal{S}_1 \sim \mathcal{S}_2$) whenever there is a simulation (resp. bisimulation) $\mathcal{R}$ such that $(q_{01}, v_{01})\mathcal{R}(q_{02}, v_{02})$, where (q_{0i}, v_{0i}) is the initial configuration of $\mathcal{S}_i$, for $i = 1, 2$.*

We say that an SRA is *complete* whenever for every configuration (p, v) and $a \in \mathcal{D}$ there is a transition $(p, v) \xrightarrow{a} (q, w)$ in $\mathsf{CLTS}(\mathcal{S})$. The following results connect similarity and language inclusion.

Proposition 1. *If $\mathcal{S}_1 \prec \mathcal{S}_2$ then $\mathscr{L}(\mathcal{S}_1) \subseteq \mathscr{L}(\mathcal{S}_2)$. If $\mathcal{S}_1$ and $\mathcal{S}_2$ are deterministic and complete, then the other direction also holds.*

It is worth noting that given a deterministic SRA we can define its *completion* by adding transitions so that every value $a \in \mathcal{D}$ can be read from any state.

Remark 1. RAs and SFAs can be encoded as SRAs on the same state-space:

- An RA is encoded as an SRA with all transition guards $\top$;
- an SFA can be encoded as an SRA with $R = \emptyset$, with each SFA transition $p \xrightarrow{\varphi} q$ encoded as $p \xrightarrow{\varphi/\emptyset,\emptyset,\emptyset} q$. Note that the absence of registers implies that the CLTS always has finitely many configurations.

SRAs are *strictly more expressive* than both RAs and SFAs. For instance, the language $\{n_0 n_1 \dots n_k \mid n_0 = n_k, \mathsf{even}(n_i), n_i \in \mathbb{Z}, i = 1, \dots, k\}$ of finite sequences of even integers where the first and last one coincide, can be recognized by an SRA, but not by an RA or by an SFA.

Boolean Closure Properties. SRAs are closed under intersection and union. Intersection is given by a standard product construction whereas union is obtained by adding a new initial state that mimics the initial states of both automata.

Proposition 2 (Closure under intersection and union). *Given SRAs* $\mathcal{S}_1$ *and* $\mathcal{S}_2$*, there are SRAs* $\mathcal{S}_1 \cap \mathcal{S}_2$ *and* $\mathcal{S}_1 \cup \mathcal{S}_2$ *such that* $\mathscr{L}(\mathcal{S}_1 \cap \mathcal{S}_2) = \mathscr{L}(\mathcal{S}_1) \cap \mathscr{L}(\mathcal{S}_2)$ *and* $\mathscr{L}(\mathcal{S}_1 \cup \mathcal{S}_2) = \mathscr{L}(\mathcal{S}_1) \cup \mathscr{L}(\mathcal{S}_2)$.

SRAs in general are not closed under complementation, because RAs are not. However, we still have closure under complementation for a subclass of SRAs.

Proposition 3. *Let* $\mathcal{S}$ *be a complete and deterministic SRA, and let* $\overline{\mathcal{S}}$ *be the SRA defined as* $\mathcal{S}$*, except that its final states are* $Q \setminus F$*. Then* $\mathscr{L}(\overline{\mathcal{S}}) = \mathcal{D}^\star \setminus \mathscr{L}(\mathcal{S})$.

4 Decidability Properties

In this section we will provide algorithms for checking determinism and emptiness for an SRA, and (bi)similarity of two SRAs. Our algorithms leverage *symbolic* techniques that use the finite syntax of SRAs to indirectly operate over the underlying configuration LTS, which can be infinite.

Single-Valued Variant. To study decidability, it is convenient to restrict register assignments to *injective* ones on non-empty registers, that is functions $v\colon R \to \mathcal{D} \cup \{\sharp\}$ such that $v(r) = v(s)$ and $v(r) \neq \sharp$ implies $r = s$. This is also the approach taken for RAs in the seminal papers [17,27]. Both for RAs and SRAs, this restriction does not affect expressivity. We say that an SRA is *single-valued* if its initial assignment v_0 is injective on non-empty registers. For single-valued SRAs, we only allow two kinds of transitions:

Read transition: $p \xrightarrow{\varphi/r^=} q$ triggers when $a \in [\![\varphi]\!]$ and a is already stored in r.
Fresh transition: $p \xrightarrow{\varphi/r^\bullet} q$ triggers when the input $a \in [\![\varphi]\!]$ and a is *fresh*, i.e., is not stored in any register. After the transition, a is stored into r.

SRAs and their single-valued variants have the same expressive power. Translating single-valued SRAs to ordinary ones is straightforward:

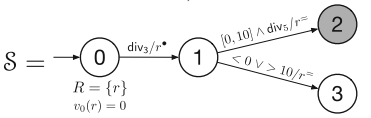
$$p \xrightarrow{\varphi/r^=} q \implies p \xrightarrow{\varphi/\{r\},\emptyset,\emptyset} q \qquad p \xrightarrow{\varphi/r^\bullet} q \implies p \xrightarrow{\varphi/\emptyset,R,\{r\}} q$$

The opposite translation requires a state-space blow up, because we need to encode register equalities in the states.

Theorem 1. *Given an SRA* $\mathcal{S}$ *with* n *states and* r *registers, there is a single-valued SRA* $\mathcal{S}'$ *with* $\mathcal{O}(nr^r)$ *states and* $r+1$ *registers such that* $\mathcal{S} \sim \mathcal{S}'$*. Moreover, the translation preserves determinism.*

Normalization. While our techniques are inspired by analogous ones for non-symbolic RAs, SRAs present an additional challenge: they can have arbitrary predicates on transitions. Hence, the values that each transition can read, and thus which configurations it can reach, depend on the history of past transitions and their predicates. This problem emerges when checking reachability and similarity, because a transition may be *disabled* by particular register values, and so lead to unsound conclusions, a problem that does not exist in register automata.

Example 3. Consider the SRA below, defined over the BA of integers.



All predicates on transitions are satisfiable, yet $\mathscr{L}(\mathcal{S}) = \emptyset$. To go from 0 to 1, $\mathcal{S}$ must read a value n such that $\mathsf{div}_3(n)$ and $n \neq 0$ and then n is stored into r. The transition from 1 to 2 can only happen if the content of r also satisfies $\mathsf{div}_5(n)$ and $n \in [0, 10]$. However, there is no n satisfying $\mathsf{div}_3(n) \wedge n \neq 0 \wedge \mathsf{div}_5(n) \wedge n \in [0, 10]$, hence the transition from 1 to 2 never happens.

To handle the complexity caused by predicates, we introduce a way of *normalizing* an SRA to an equivalent one that *stores additional information about input predicates*. We first introduce some notation and terminology.

A register abstraction θ for $\mathcal{S}$, used to "keep track" of the domain of registers, is a family of predicates indexed by the registers R of $\mathcal{S}$. Given a register assignment v, we write $v \models \theta$ whenever $v(r) \in [\![\theta_r]\!]$ for $v(r) \neq \sharp$, and $\theta_r = \bot$ otherwise. Hereafter we shall only consider "meaningful" register abstractions, for which there is at least one assignment v such that $v \models \theta$.

With the contextual information about register domains given by θ, we say that a transition $p \xrightarrow{\varphi/\ell} q \in \Delta$ is *enabled by* θ whenever it has at least an instance $(p, v) \xrightarrow{a} (q, w)$ in $\mathsf{CLTS}(\mathcal{S})$, for all $v \models \theta$. Enabled transitions are important when reasoning about reachability and similarity.

Checking whether a transition has at least one realizable instance in the CLTS is difficult in practice, especially when $\ell = r^\bullet$, because it amounts to checking whether $[\![\varphi]\!] \setminus \mathsf{img}(v) \neq \emptyset$, for all injective $v \models \theta$.

To make the check for enabledness practical we will use minterms. For a set of predicates Φ, a *minterm* is a minimal satisfiable Boolean combination of all predicates that occur in Φ. Minterms are the analogue of atoms in a complete atomic Boolean algebra. E.g. the set of predicates $\Phi = \{x > 2, x < 5\}$ over the theory of linear integer arithmetic has minterms $\mathsf{mint}(\Phi) = \{x > 2 \wedge x < 5,\ \neg x > 2 \wedge x < 5,\ x > 2 \wedge \neg x < 5\}$. Given $\psi \in \mathsf{mint}(\Phi)$ and $\varphi \in \Phi$, we will write $\varphi \sqsubset \psi$ whenever φ appears non-negated in ψ, for instance $(x > 2) \sqsubset (x > 2 \wedge \neg x < 5)$. A crucial property of minterms is that they do not overlap, i.e., $\mathsf{isSat}(\psi_1 \wedge \psi_2)$ if and only if $\psi_1 = \psi_2$, for ψ_1 and ψ_2 minterms.

Lemma 1 (Enabledness). *Let θ be a register abstraction such that θ_r is a minterm, for all $r \in R$. If φ is a minterm, then $p \xrightarrow{\varphi/\ell} q$ is enabled by θ iff:*

(1) if $\ell = r^{=}$*, then* $\varphi = \theta_r$*;* *(2) if* $\ell = r^{\bullet}$*, then* $|[\![\varphi]\!]| > \mathscr{E}(\theta, \varphi)$*,*
where $\mathscr{E}(\theta, \varphi) = |\{r \in R \mid \theta_r = \varphi\}|$ *is the # of registers with values from* $[\![\varphi]\!]$*.*

Intuitively, (1) says that if the transition reads a symbol stored in r satisfying φ, the symbol must also satisfy θ_r, the range of r. Because φ and θ_r are minterms, this only happens when $\varphi = \theta_r$. (2) says that the enabling condition $[\![\varphi]\!] \setminus \mathsf{img}(v) \neq \emptyset$, for all injective $v \models \theta$, holds if and only if there are fewer registers storing values from φ than the cardinality of φ. That implies we can always find a fresh element in $[\![\varphi]\!]$ to enable the transition. Registers holding values from φ are exactly those $r \in R$ such that $\theta_r = \varphi$. Both conditions can be effectively checked: the first one is a simple predicate-equivalence check, while the second one amounts to checking whether φ holds for at least a certain number k of distinct elements. This can be achieved by checking satisfiability of $\varphi \wedge \neg\mathsf{atom}(a_1) \wedge \cdots \wedge \neg\mathsf{atom}(a_{k-1})$, for $a_1, \ldots, a_{k-1}$ distinct elements of $[\![\varphi]\!]$.

Remark 2. Using single-valued SRAs to check enabledness might seem like a restriction. However, if one would start from a generic SRA, the process to check enabledness would contain an extra step: for each state p, we would have to keep track of all possible equations among registers. In fact, register equalities determine whether (i) register constraints of an outgoing transition are satisfiable; (ii) how many elements of the guard we need for the transition to happen, analogously to condition 2 of Lemma 1. Generating such equations is the key idea behind Theorem 1, and corresponds precisely to turning the SRA into a single-valued one.

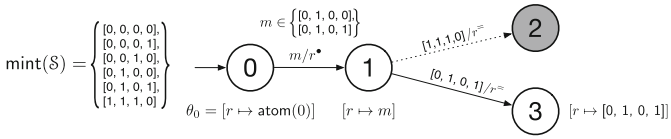
Given any SRA, we can use the notion of register abstraction to build an equivalent *normalized* SRA, where (i) states keep track of how the domains of registers change along transitions, (ii) transitions are obtained by breaking the one of the original SRA into minterms and discarding the ones that are disabled according to Lemma 1. In the following we write $\mathsf{mint}(\mathcal{S})$ for the minterms for the set of predicates $\{\varphi \mid p \xrightarrow{\varphi/\ell} q \in \Delta\} \cup \{\mathsf{atom}(v_0(r)) \mid v_0(r) \in \mathcal{D}, r \in R\}$. Observe that an atomic predicate always has an equivalent minterm, hence we will use atomic predicates to define the initial register abstraction.

Definition 4 (Normalized SRA). *Given an SRA* $\mathcal{S}$*, its normalization* $\mathsf{N}(\mathcal{S})$ *is the SRA* $(R, \mathsf{N}(Q), \mathsf{N}(q_0), v_0, \mathsf{N}(F), \mathsf{N}(\Delta))$ *where:*

- $\mathsf{N}(Q) = \{\theta \mid \theta$ *is a register abstraction over* $\mathsf{mint}(\mathcal{S}) \cup \{\bot\}\} \times Q$*; we will write* $\theta \rhd q$ *for* $(\theta, q) \in \mathsf{N}(Q)$*.*
- $\mathsf{N}(q_0) = \theta_0 \rhd q_0$*, where* $(\theta_0)_r = \mathsf{atom}(v_0(r))$ *if* $v_0(r) \in \mathcal{D}$*, and* $(\theta_0)_r = \bot$ *if* $v_0(r) = \sharp$*;*
- $\mathsf{N}(F) = \{\theta \rhd p \in \mathsf{N}(Q) \mid p \in F\}$
- $\mathsf{N}(\Delta) = \{\theta \rhd p \xrightarrow{\theta_r/r^{=}} \theta \rhd q \mid p \xrightarrow{\varphi/r^{=}} q \in \Delta, \varphi \sqsubset \theta_r\} \cup$
  $\{\theta \rhd p \xrightarrow{\psi/r^{\bullet}} \theta[r \mapsto \psi] \rhd q \mid p \xrightarrow{\varphi/r^{\bullet}} q \in \Delta, \varphi \sqsubset \psi, |[\![\psi]\!]| > \mathscr{E}(\theta, \psi)\}$

The automaton $\mathsf{N}(\mathcal{S})$ enjoys the desired property: each transition from $\theta \rhd p$ is enabled by θ, by construction. $\mathsf{N}(\mathcal{S})$ is always *finite*. In fact, suppose $\mathcal{S}$ has n states, m transitions and r registers. Then $\mathsf{N}(\mathcal{S})$ has at most m predicates, and $|\mathsf{mint}(\mathcal{S})|$ is $\mathcal{O}(2^m)$. Since the possible register abstractions are $\mathcal{O}(r2^m)$, $\mathsf{N}(\mathcal{S})$ has $\mathcal{O}(nr2^m)$ states and $\mathcal{O}(mr^2 2^{3m})$ transitions.

Example 4. We now show the normalized version of Example 3. The first step is computing the set $\mathsf{mint}(\mathcal{S})$ of minterms for $\mathcal{S}$, i.e., the satisfiable Boolean combinations of $\{\mathsf{atom}(0), \mathsf{div}_3, [0,10] \wedge \mathsf{div}_5, < 0 \vee > 10\}$. For simplicity, we represent minterms as bitvectors where a 0 component means that the corresponding predicate is negated, e.g., $[1,1,1,0]$ stands for the minterm $\mathsf{atom}(0) \wedge ([0,10] \wedge \mathsf{div}_3) \wedge \mathsf{div}_5 \wedge \neg(< 0 \vee > 10)$. Minterms and the resulting SRA $\mathsf{N}(\mathcal{S})$ are shown below.



On each transition we show how it is broken down to minterms, and for each state we show the register abstraction (note that state 1 becomes two states in $\mathsf{N}(\mathcal{S})$). The transition from 1 to 2 is *not* part of $\mathsf{N}(\mathcal{S})$ – this is why it is dotted. In fact, in every register abstraction $[r \mapsto m]$ reachable at state 1, the component for the transition guard $[0,10] \wedge \mathsf{div}_5$ in the minterm m (3rd component) is 0, i.e., $([0,10] \wedge \mathsf{div}_5) \not\sqsubseteq m$. Intuitively, this means that r will never be assigned a value that satisfies $[0,10] \wedge \mathsf{div}_5$. As a consequence, the construction of Definition 4 will not add a transition from 1 to 2.

Finally, we show that the normalized SRA behaves exactly as the original one.

Proposition 4. *$(p, v) \sim (\theta \rhd p, v)$, for all $p \in Q$ and $v \models \theta$. Hence, $\mathcal{S} \sim \mathsf{N}(\mathcal{S})$.*

Emptiness and Determinism. The transitions of $\mathsf{N}(\mathcal{S})$ are always enabled by construction, therefore every path in $\mathsf{N}(\mathcal{S})$ always corresponds to a run in $\mathsf{CLTS}(\mathsf{N}(\mathcal{S}))$.

Lemma 2. *The state $\theta \rhd p$ is reachable in $\mathsf{N}(\mathcal{S})$ if and only if there is a reachable configuration $(\theta \rhd p, v)$ in $\mathsf{CLTS}(\mathsf{N}(\mathcal{S}))$ such that $v \models \theta$. Moreover, if $(\theta \rhd p, v)$ is reachable, then all configurations $(\theta \rhd p, w)$ such that $w \models \theta$ are reachable.*

Therefore, using Proposition 4, we can reduce the reachability and emptiness problems of $\mathcal{S}$ to that of $\mathsf{N}(\mathcal{S})$.

Theorem 2 (Emptiness). *There is an algorithm to decide reachability of any configuration of $\mathcal{S}$, hence whether $\mathscr{L}(\mathcal{S}) = \emptyset$.*

Proof. Let (p, v) be a configuration of $\mathcal{S}$. To decide whether it is reachable in $\mathsf{CLTS}(\mathcal{S})$, we can perform a visit of $\mathsf{N}(\mathcal{S})$ from its initial state, stopping when a

state $\theta \triangleright p$ such that $v \models \theta$ is reached. If we are just looking for a final state, we can stop at any state such that $p \in F$. In fact, by Proposition 4, there is a run in $\mathsf{CLTS}(\mathcal{S})$ ending in (p, v) if and only if there is a run in $\mathsf{CLTS}(\mathsf{N}(\mathcal{S}))$ ending in $(\theta \triangleright p, v)$ such that $v \models \theta$. By Lemma 2, the latter holds if and only if there is a path in $\mathsf{N}(\mathcal{S})$ ending in $\theta \triangleright p$. This algorithm has the complexity of a standard visit of $\mathsf{N}(\mathcal{S})$, namely $\mathcal{O}(nr2^m + mr^2 2^{3m})$. □

Now that we characterized which transitions are reachable, we define what it means for a normalized SRA to be deterministic and we show that determinism is preserved by the translation from SRA.

Proposition 5 (Determinism). $\mathsf{N}(\mathcal{S})$ *is* deterministic *if and only if for all reachable transitions* $p \xrightarrow{\varphi_1/\ell_1} q_1, p \xrightarrow{\varphi_2/\ell_2} q_2 \in \mathsf{N}(\Delta)$ *the following holds:* $\varphi_1 \neq \varphi_2$ *whenever either (1)* $\ell_1 = \ell_2$ *and* $q_1 \neq q_2$*, or; (2)* $\ell_1 = r^\bullet$*,* $\ell_2 = s^\bullet$*, and* $r \neq s$*;*

One can check determinism of an SRA by looking at its normalized version.

Proposition 6. $\mathcal{S}$ *is deterministic if and only if* $\mathsf{N}(\mathcal{S})$ *is deterministic.*

Similarity and Bisimilarity. We now introduce a symbolic technique to decide similarity and bisimilarity of SRAs. The basic idea is similar to *symbolic (bi)simulation* [20,27] for RAs. Recall that RAs are SRAs whose transition guards are all $\top$. Given two RAs $\mathcal{S}_1$ and $\mathcal{S}_2$ a symbolic simulation between them is defined over their state spaces Q_1 and Q_2, not on their configurations. For this to work, one needs to add an extra piece of information about how registers of the two states are related. More precisely, a symbolic simulation is a relation on triples (p_1, p_2, σ), where $p_1 \in Q_1, p_2 \in Q_2$ and $\sigma \subseteq R_1 \times R_2$ is a *partial injective* function. This function encodes constraints between registers: $(r, s) \in \sigma$ is an equality constraint between $r \in R_1$ and $s \in R_2$, and $(r, s) \notin \sigma$ is an inequality constraint. Intuitively, (p_1, p_2, σ) says that all configurations (p_1, v_1) and (p_2, v_2) such that v_1 and v_2 satisfy σ – e.g., $v_1(r) = v_2(s)$ whenever $(r, s) \in \sigma$ – are in the simulation relation $(p_1, v_1) \prec (p_2, v_2)$. In the following we will use $v_1 \bowtie v_2$ to denote the function encoding constraints among v_1 and v_2, explicitly: $\sigma(r) = s$ if and only if $v_1(r) = v_2(s)$ and $v_1(r) \neq \sharp$.

Definition 5 (Symbolic (bi)similarity [27]). *A symbolic simulation is a relation* $\mathcal{R} \subseteq Q_1 \times Q_1 \times \mathcal{P}(R_1 \times R_2)$ *such that if* $(p_1, p_2, \sigma) \in \mathcal{R}$*, then* $p_1 \in F_1$ *implies* $p_2 \in F_2$*, and if* $p_1 \xrightarrow{\ell} q_1 \in \Delta_1$[1] *then:*

1. *if* $\ell = r^=$*:*
   (a) *if* $r \in \mathsf{dom}(\sigma)$*, then there is* $p_2 \xrightarrow{\sigma(r)^=} q_2 \in \Delta_2$ *such that* $(q_1, q_2, \sigma) \in \mathcal{R}$*.*
   (b) *if* $r \notin \mathsf{dom}(\sigma)$ *then there is* $p_2 \xrightarrow{s^\bullet} q_2 \in \Delta_2$ *s.t.* $(q_1, q_2, \sigma[r \mapsto s]) \in \mathcal{R}$*.*

[1] We will keep the $\top$ guard implicit for succinctness.

2 if $\ell = r^\bullet$*:*

(a) for all $s \in R_2 \setminus \mathsf{img}(\sigma)$*, there is* $p_2 \xrightarrow{s^=} q_2 \in \Delta_2$ *such that* $(q_1, q_2, \sigma[r \mapsto s]) \in \mathcal{R}$*, and;*

(b) there is $p_2 \xrightarrow{s^\bullet} q_2 \in \Delta_2$ *such that* $(q_1, q_2, \sigma[r \mapsto s]) \in \mathcal{R}$*.*

Here $\sigma[r \mapsto s]$ *stands for* $\sigma \setminus (\sigma^{-1}(s), s) \cup (r, s)$*, which ensures that* σ *stays injective when updated.*

Given a symbolic simulation $\mathcal{R}$*, its inverse is defined as* $\mathcal{R}^{-1} = \{t^{-1} \mid t \in \mathcal{R}\}$*, where* $(p_1, p_2, \sigma)^{-1} = (p_2, p_1, \sigma^{-1})$*. A* symbolic bisimulation $\mathcal{R}$ *is a relation such that both* $\mathcal{R}$ *and* $\mathcal{R}^{-1}$ *are symbolic simulations.*

Case 1 deals with cases when p_1 can perform a transition that reads the register r. If $r \in \mathsf{dom}(\sigma)$, meaning that r and $\sigma(r) \in R_2$ contain the same value, then p_2 must be able to read $\sigma(r)$ as well. If $r \notin \mathsf{dom}(\sigma)$, then the content of r is fresh w.r.t. p_2, so p_2 must be able to read any fresh value—in particular the content of r. Case 2 deals with the cases when p_1 reads a fresh value. It ensures that p_2 is able to read all possible values that are fresh for p_1, be them already in some register s – i.e., $s \in R_2 \setminus \mathsf{img}(\sigma)$, case 2(a) – or fresh for p_2 as well – case 2(b). In all these cases, σ must be updated to reflect the new equalities among registers.

Keeping track of equalities among registers is enough for RAs, because the actual content of registers does not determine the capability of a transition to fire (RA transitions have implicit $\top$ guards). As seen in Example 3, this is no longer the case for SRAs: a transition may or may not happen depending on the register assignment being compatible with the transition guard.

As in the case of reachability, normalized SRAs provide the solution to this problem. We will reduce the problem of checking (bi)similarity of $\mathcal{S}_1$ and $\mathcal{S}_2$ to that of checking symbolic (bi)similarity on $\mathsf{N}(\mathcal{S}_1)$ and $\mathsf{N}(\mathcal{S}_2)$, with minor modifications to the definition. To do this, we need to assume that minterms for both $\mathsf{N}(\mathcal{S}_1)$ and $\mathsf{N}(\mathcal{S}_2)$ are computed over the union of predicates of $\mathcal{S}_1$ and $\mathcal{S}_2$.

Definition 6 (N-simulation). *A N-simulation on* $\mathcal{S}_1$ *and* $\mathcal{S}_2$ *is a relation* $\mathcal{R} \subseteq \mathsf{N}(Q_1) \times \mathsf{N}(Q_2) \times \mathcal{P}(R_1 \times R_2)$*, defined as in Definition 5, with the following modifications:*

(i) we require that $\theta_1 \rhd p_1 \xrightarrow{\varphi_1/\ell_1} \theta_1' \rhd q_1 \in \mathsf{N}(\Delta_1)$ *must be matched by transitions* $\theta_2 \rhd p_2 \xrightarrow{\varphi_2/\ell_2} \theta_2' \rhd q_2 \in \mathsf{N}(\Delta_2)$ *such that* $\varphi_2 = \varphi_1$*.*

(ii) we modify case 2 as follows (changes are underlined):

2(a)' for all $s \in R_2 \setminus \mathsf{img}(\sigma)$ *such that* $\varphi_1 = (\theta_2)_s$*, there is* $\theta_2 \rhd p_2 \xrightarrow{\varphi_1/s^=} \theta_2' \rhd q_2 \in \mathsf{N}(\Delta_2)$ *such that* $(\theta_1' \rhd q_1, \theta_2' \rhd q_2, \sigma[r \mapsto s]) \in \mathcal{R}$*, and;*

2(b)' if $\mathscr{E}(\theta_1, \varphi_1) + \mathscr{E}(\theta_2, \varphi_1) < |[\![\varphi_1]\!]|$*, then there is* $\theta_2 \rhd p_2 \xrightarrow{\varphi_1/s^\bullet} \theta_2' \rhd q_2 \in \mathsf{N}(\Delta_2)$ *such that* $(\theta_1' \rhd q_1, \theta_2' \rhd q_2, \sigma[r \mapsto s]) \in \mathcal{R}$*.*

A N-bisimulation $\mathcal{R}$ *is a relation such that both* $\mathcal{R}$ *and* $\mathcal{R}^{-1}$ *are N-simulations. We write* $\mathcal{S}_1 \overset{\mathsf{N}}{\prec} \mathcal{S}_2$ *(resp.* $\mathcal{S}_1 \overset{\mathsf{N}}{\sim} \mathcal{S}_2$*) if there is a N-simulation (resp. bisimulation)* $\mathcal{R}$ *such that* $(\mathsf{N}(q_{01}), \mathsf{N}(q_{02}), v_{01} \bowtie v_{02}) \in \mathcal{R}$*.*

The intuition behind this definition is as follows. Recall that, in a normalized SRA, transitions are defined over minterms, which cannot be further broken down, and are mutually disjoint. Therefore two transitions can read the same values if and only if they have the same minterm guard. Thus condition (i) makes sure that matching transitions can read exactly the same set of values. Analogously, condition (ii) restricts how a fresh transition of $\mathsf{N}(\mathcal{S}_1)$ must be matched by one of $\mathsf{N}(\mathcal{S}_2)$: 2(a)' only considers transitions of $\mathsf{N}(\mathcal{S}_2)$ reading registers $s \in R_2$ such that $\varphi_1 = (\theta_2)_s$ because, by definition of normalized SRA, $\theta_2 \rhd p_2$ has no such transition if this condition is not met. Condition 2(b)' amounts to requiring a fresh transition of $\mathsf{N}(\mathcal{S}_2)$ that is enabled by both θ_1 and θ_2 (see Lemma 1), i.e., that can read a symbol that is fresh w.r.t. both $\mathsf{N}(\mathcal{S}_1)$ and $\mathsf{N}(\mathcal{S}_2)$.

N-simulation is sound and complete for standard simulation.

Theorem 3. *$\mathcal{S}_1 \prec \mathcal{S}_2$ if and only if $\mathcal{S}_1 \overset{\mathsf{N}}{\prec} \mathcal{S}_2$.*

As a consequence, we can decide similarity of SRAs via their normalized versions. N-simulation is a relation over a finite set, namely $\mathsf{N}(Q_1) \times \mathsf{N}(Q_2) \times \mathcal{P}(R_1 \times R_2)$, therefore N-similarity can always be decided in finite time. We can leverage this result to provide algorithms for checking language inclusion/equivalence for deterministic SRAs (recall that they are undecidable for non-deterministic ones).

Theorem 4. *Given two deterministic SRAs $\mathcal{S}_1$ and $\mathcal{S}_2$, there are algorithms to decide $\mathscr{L}(\mathcal{S}_1) \subseteq \mathscr{L}(\mathcal{S}_2)$ and $\mathscr{L}(\mathcal{S}_1) = \mathscr{L}(\mathcal{S}_2)$.*

Proof. By Proposition 1 and Theorem 3, we can decide $\mathscr{L}(\mathcal{S}_1) \subseteq \mathscr{L}(\mathcal{S}_2)$ by checking $\mathcal{S}_1 \overset{\mathsf{N}}{\prec} \mathcal{S}_2$. This can be done algorithmically by iteratively building a relation $\mathcal{R}$ on triples that is an N-simulation on $\mathsf{N}(\mathcal{S}_1)$ and $\mathsf{N}(\mathcal{S}_2)$. The algorithm initializes $\mathcal{R}$ with $(\mathsf{N}(q_{01}), \mathsf{N}(q_{02}),\ v_{01} \bowtie v_{02})$, as this is required to be in $\mathcal{R}$ by Definition 6. Each iteration considers a candidate triple t and checks the conditions for N-simulation. If satisfied, it adds t to $\mathcal{R}$ and computes the next set of candidate triples, i.e., those which are required to belong to the simulation relation, and adds them to the list of triples still to be processed. If not, the algorithm returns $\mathscr{L}(\mathcal{S}_1) \not\subseteq \mathscr{L}(\mathcal{S}_2)$. The algorithm terminates returning $\mathscr{L}(\mathcal{S}_1) \subseteq \mathscr{L}(\mathcal{S}_2)$ when no triples are left to process. Determinism of $\mathcal{S}_1$ and $\mathcal{S}_2$, and hence of $\mathsf{N}(\mathcal{S}_1)$ and $\mathsf{N}(\mathcal{S}_2)$ (by Proposition 6), ensures that computing candidate triples is deterministic. To decide $\mathscr{L}(\mathcal{S}_1) = \mathscr{L}(\mathcal{S}_2)$, at each iteration we need to check that both t and t^{-1} satisfy the conditions for N-simulation.

If $\mathcal{S}_1$ and $\mathcal{S}_2$ have, respectively, n_1, n_2 states, m_1, m_2 transitions, and r_1, r_2 registers, the normalized versions have $\mathcal{O}(n_1 r_1 2^{m_1})$ and $\mathcal{O}(n_2 r_2 2^{m_2})$ states. Each triple, taken from the finite set $\mathsf{N}(Q_1) \times \mathsf{N}(Q_2) \times \mathcal{P}(R_1 \times R_2)$, is processed exactly once, so the algorithm iterates $\mathcal{O}(n_1 n_2 r_1 r_2 2^{m_1+m_2+r_1 r_2})$ times. □

5 Evaluation

We have implemented SRAs in the open-source Java library SVPALib [26]. In our implementation, constructions are computed lazily when possible (e.g., the

normalized SRA for emptiness and (bi)similarity checks). All experiments were performed on a machine with 3.5 GHz Intel Core i7 CPU with 16 GB of RAM (JVM 8 GB), with a timeout value of 300 s. The goal of our evaluation is to answer the following research questions:

Q1: Are SRAs more succinct than existing models when processing strings over large but finite alphabets? (Sect. 5.1)
Q2: What is the performance of membership for deterministic SRAs and how does it compare to the matching algorithm in `java.util.regex`? (Sect. 5.2)
Q3: Are SRA decision procedures practical? (Sect. 5.3)

Benchmarks. We focus on regular expressions with back-references, therefore all our benchmarks operate over the Boolean algebra of Unicode characters with interval—i.e., the set of characters is the set of all 2^{16} UTF-16 characters and the predicates are union of intervals (e.g., `[a-zA-Z]`).[2] Our benchmark set contains 19 SRAs that represent variants of regular expressions with back-references obtained from the regular-expression crowd-sourcing website RegExLib [23]. The expressions check whether inputs have, for example, matching first/last name initials or both (Name-F, Name-L and Name), correct Product Codes/Lot number of total length n (Pr-Cn, Pr-CLn), matching XML tags (XML), and IP addresses that match for n positions (IPn). We also create variants of the product benchmark presented in Sect. 2 where we vary the numbers of characters in the code and lot number. All the SRAs are deterministic.

5.1 Succinctness of SRAs vs SFAs

In this experiment, we relate the size of SRAs over finite alphabets to the size of the smallest equivalent SFAs. For each SRA, we construct the equivalent SFA by equipping the state space with the values stored in the registers at each step (this construction effectively builds the configuration LTS). Figure 2a shows the results. As expected, SFAs tend to blow up in size when the SRA contains multiple registers or complex register values. In cases where the register values range over small sets (e.g., `[0-9]`) it is often feasible to build an SFA equivalent to the SRA, but the construction always yields very large automata. In cases where the registers can assume many values (e.g., 2^{16}) SFAs become prohibitively large and do not fit in memory. To answer **Q1**, even for finite alphabets, **it is not feasible to compile SRAs to SFAs**. Hence, SRAs are a succinct model.

5.2 Performance of Membership Checking

In this experiment, we measure the performance of SRA membership, and we compare it with the performance of the `java.util.regex` matching algorithm.

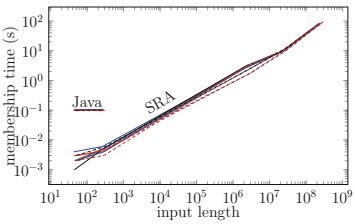
[2] Our experiments are over finite alphabets, but the Boolean algebra can be infinite by taking the alphabet to be positive integers and allowing intervals to contain ∞ as upper bound. This modification does not affect the running time of our procedures, therefore we do not report it.

	SRA				SFA	
	states	tr	reg	|reg|	states	tr
IP2	44	46	3	10	4,013	4,312
IP3	44	46	4	10	39,113	42,112
IP4	44	46	5	10	372,113	402,112
IP6	44	46	7	10	—	—
IP9	44	46	10	10	—	—
Name-F	7	10	2	26	201	300
Name-L	7	10	2	26	129	180
Name	7	10	3	26	3,201	4,500
XML	12	16	4	52	—	—
Pr-C2	26	28	3	2^{16}	—	—
Pr-C3	28	30	4	2^{16}	—	—
Pr-C4	30	32	5	2^{16}	—	—
Pr-C6	34	36	7	2^{16}	—	—
Pr-C9	40	42	10	2^{16}	—	—
Pr-CL2	26	28	3	2^{16}	—	—
Pr-CL3	28	30	4	2^{16}	—	—
Pr-CL4	30	32	5	2^{16}	—	—
Pr-CL6	34	36	7	2^{16}	—	—
Pr-CL9	40	42	10	2^{16}	—	—

(a) Size of SRAs vs SFAs. (—) denotes the SFA didn't fit in memory. |reg| denotes how many different characters a register stored.

SRA $\mathcal{S}_1$	SRA $\mathcal{S}_2$	$\mathscr{L}_1 = \emptyset$	$\mathscr{L}_1 = \mathscr{L}_1$	$\mathscr{L}_2 \subseteq \mathscr{L}_1$
Pr-C2	Pr-CL2	0.125s	0.905s	3.426s
Pr-C3	Pr-CL3	1.294s	5.558s	24.688s
Pr-C4	Pr-CL4	13.577s	55.595s	—
Pr-C6	Pr-CL6	—	—	—
Pr-CL2	Pr-C2	1.067s	0.952s	0.889s
Pr-CL3	Pr-C3	10.998s	11.104s	11.811s
Pr-CL4	Pr-C4	—	—	—
Pr-CL6	Pr-C6	—	—	—
IP-2	IP-3	0.125s	0.408s	1.845s
IP-3	IP-4	1.288s	2.953s	21.627s
IP-4	IP-6	18.440s	42.727s	—
IP-6	IP-9	—	—	—

(b) Performance of decision procedures. In the table $\mathscr{L}_i = \mathscr{L}(\mathcal{S}_i)$, for $i = 1, 2$.



(c) SRA membership and Java `regex` matching performance. Missing data points for Java are stack overflows.

Fig. 2. Experimental results.

For each benchmark, we generate inputs of length varying between approximately 100 and 10^8 characters and measure the time taken to check membership. Figure 2c shows the results. The performance of SRA (resp. Java) is not particularly affected by the size of the expression. Hence, the lines for different expressions mostly overlap. As expected, for SRAs the time taken to check membership grows linearly in the size of the input (axes are log scale). Remarkably, even though our implementation does not employ particular input processing optimizations, it can still check membership for strings with tens of millions of characters in less than 10 s. We have found that our implementation is more efficient than the Java `regex` library, matching the same input an average of 50 times faster than `java.util.regex.Matcher`. `java.util.regex.Matcher` seems to make use of a recursive algorithm to match back-references, which means it does not scale well. Even when given the maximum stack size, the JVM will return a Stack Overflow for inputs as small as 20,000 characters. Our implementation can match such strings in less than 2 s. To answer **Q2**, **deterministic SRAs can be efficiently executed on large inputs and perform better than the `java.util.regex` matching algorithm**.

5.3 Performance of Decision Procedures

In this experiment, we measure the performance of SRAs simulation and bisimulation algorithms. Since all our SRAs are deterministic, these two checks correspond to language equivalence and inclusion. We select pairs of benchmarks for which the above tests are meaningful (e.g., variants of the problem discussed at the end of Sect. 2). The results are shown in Fig. 2b. As expected, due to the translation to single-valued SRAs, our decision procedures do not scale well in the number of registers. This is already the case for classic register automata and it is not a surprising result. However, our technique can still check equivalence and inclusion for regular expressions that no existing tool can handle. To answer **Q3**, **bisimulation and simulation algorithms for SRAs only scale to small numbers of registers**.

6 Conclusions

In this paper we have presented *Symbolic Register Automata*, a novel class of automata that can handle complex alphabet theories while allowing symbol comparisons for equality. SRAs encompass – and are strictly more powerful – than both Register and Symbolic Automata. We have shown that they enjoy the same closure and decidability properties of the former, despite the presence of arbitrary guards on transitions, which are not allowed by RAs. Via a comprehensive set of experiments, we have concluded that SRAs are vastly more succinct than SFAs and membership is efficient on large inputs. Decision procedures do not scale well in the number of registers, which is already the case for basic RAs.

Related Work. RAs were first introduced in [17]. There is an extensive literature on register automata, their formal languages and decidability properties [7,13,21,22,25], including variants with *global freshness* [20,27] and totally ordered data [4,14]. SRAs are based on the original model of [17], but are much more expressive, due to the presence of guards from an arbitrary decidable theory.

In recent work, variants over richer theories have appeared. In [9] RA over rationals were introduced. They allow for a restricted form of linear arithmetic among registers (RAs with arbitrary linear arithmetic subsume two-counter automata, hence are undecidable). SRAs do not allow for operations on registers, but encompass a wider range of theories without any loss in decidability. Moreover, [9] does not study Boolean closure properties. In [8,16], RAs allowing guards over a range of theories – including (in)equality, total orders and increments/sums – are studied. Their focus is different than ours as they are interested primarily in *active learning* techniques, and several restrictions are placed on models for the purpose of the learning process. We can also relate SRAs with *Quantified Event Automata* [2], which allow for guards and assignments to registers on transitions. However, in QEA guards can be arbitrary, which could lead to several problems, e.g. undecidable equivalence.

Symbolic automata were first introduced in [28] and many variants of them have been proposed [12]. The one that is closer to SRAs is Symbolic Extended Finite Automata (SEFA) [11]. SEFAs are SFAs in which transitions can read more than one character at a time. A transition of arity k reads k symbols which are consumed if they satisfy the predicate $\varphi(x_1, \ldots, x_k)$. SEFAs allow arbitrary k-ary predicates over the input theory, which results in most problems being undecidable (e.g., equivalence and intersection emptiness) and in the model not being closed under Boolean operations. Even when deterministic, SEFAs are not closed under union and intersection. In terms of expressiveness, SRAs and SEFAs are incomparable. SRAs can only use equality, but can compare symbols at arbitrary points in the input while SEFAs can only compare symbols within a constant window, but using arbitrary predicates.

Several works study matching techniques for extended regular expressions [3,5,18,24]. These works introduce automata models with ad-hoc features for extended regular constructs – including back-references – but focus on efficient matching, without studying closure and decidability properties. It is also worth noting that SRAs are not limited to alphanumeric or finite alphabets. On the negative side, SRAs cannot express capturing groups of an unbounded length, due to the finitely many registers. This limitation is essential for decidability.

Future Work. In [21] a polynomial algorithm for checking language equivalence of deterministic RAs is presented. This crucially relies on closure properties of symbolic bisimilarity, some of which are lost for SRAs. We plan to investigate whether this algorithm can be adapted to our setting. Extending SRAs with more complex comparison operators other than equality (e.g., a total order $<$) is an interesting research question, but most extensions of the model quickly lead to undecidability. We also plan to study active automata learning for SRAs, building on techniques for SFAs [1], RAs [6,8,16] and nominal automata [19].

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Abstraction Refinement Algorithms for Timed Automata

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Abstract. We present abstraction-refinement algorithms for model checking safety properties of timed automata. The abstraction domain we consider abstracts away zones by restricting the set of clock constraints that can be used to define them, while the refinement procedure computes the set of constraints that must be taken into consideration in the abstraction so as to exclude a given spurious counterexample. We implement this idea in two ways: an enumerative algorithm where a lazy abstraction approach is adopted, meaning that possibly different abstract domains are assigned to each exploration node; and a symbolic algorithm where the abstract transition system is encoded with Boolean formulas.

1 Introduction

Model checking [4,10,12,26] is an automated technique for verifying that the set of behaviors of a computer system satisfies a given property. Model-checking algorithms explore finite-state automata (representing the system under study) in order to decide if the property holds; if not, the algorithm returns an explanation. These algorithms have been extended to verify real-time systems modelled as timed automata [2,3], an extension of finite automata with clock variables to measure and constrain the amount of time elapsed between occurrences of transitions. The state-space exploration can be done by representing clock constraints efficiently using convex polyhedra called *zones* [8,9]. Algorithms based on this data structure have been implemented in several tools such as Uppaal [7], and have been applied in various industrial cases.

The well-known issue in the applications of model checking is the *state-space explosion* problem: the size of the state space grows exponentially in the size of the description of the system. There are several sources for this explosion: the system might be made of the composition of several subsystems (such as a distributed system), it might contain several discrete variables (such as in a piece of software), or it might contain a number of real-valued clocks as in our case.

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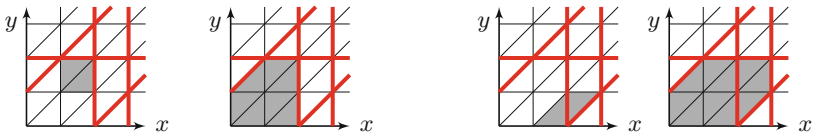
Numerous attempts have been made to circumvent this problem. Abstraction is a generic approach that consists in simplifying the model under study, so as to make it easier to verify [13]. *Existential* abstraction may only add extra behaviors, so that when a safety property holds in an abstracted model, it also holds in the original model; if on the other hand a safety property fails to hold, the model-checking algorithms return a witness trace exhibiting the non-safe behaviour: this either invalidates the property on the original model, if the trace exists in that model, or gives information about how to automatically refine the abstraction. This approach, named CEGAR (counter-example guided abstraction refinement) [11], was further developed and used, for instance, in software verification (BLAST [20], SLAM [5], ...).

The CEGAR approach has been adapted to timed automata, e.g. in [14, 18], but the abstractions considered there only consist in removing clocks and discrete variables, and adding them back during refinement. So for most well-designed models, one ends up adding all clocks and variables which renders the method useless. Two notable exceptions are [22], in which the zone extrapolation operators are dynamically adapted during the exploration, and [29], in which zones are refined when needed using interpolants. Both approaches define "exact" abstractions in the sense that they make sure that all traces discovered in the abstract model are feasible in the concrete model at any time.

In this work, we consider a more general setting and study *predicate abstractions* on clock variables. Just like in software model checking, we define abstract state spaces using these predicates, where the values of the clocks and their relations are approximately represented by these predicates. New predicates are generated if needed during the refinement step. We instantiate our approach by two algorithms. The first one is a zone-based enumerative algorithm inspired by the *lazy abstraction* in software model checking [19], where we assign a possibly different abstract domain to each node in the exploration. The second algorithm is based on binary decision diagrams (BDD): by exploiting the observation that a small number of predicates was often sufficient to prove safety properties, we use an efficient BDD encoding of zones similar to one introduced in early work [28].

Let us explain the abstract domains we consider. Assume there are two clock variables x and y. The abstraction we consider consists in restricting the clock



(a) Abstraction of zone $1 \leq x, y \leq 2$ (b) Abstraction of zone $y \leq 1 \wedge 1 \leq x - y \leq 2$

Fig. 1. The abstract domain is defined by the clock constraints shown in thick red lines. In each example, the abstraction of the zone shown on the left (shaded area) is the larger zone on the right. (Color figure online)

constraints that can be used when defining zones. Assume that we only allow to compare x with 2 or 3; that y can only be compared with 2, and $x-y$ can only be compared with -1 or 2. Then any conjunction of constraints one might obtain in this manner will be delimited by the thick red lines in Fig. 1; one cannot define a finer region under this restriction. The figure shows the abstraction process: given a "concrete" zone, its abstraction is the smallest zone which is a superset and is definable under our restriction. For instance, the abstraction of $1 \leq x, y \leq 2$ is $0 \leq x, y \leq 2 \wedge -1 \leq x - y$ (cf. Fig. 1a).

Related Works. We give more detail on zone abstractions in timed automata. Most efforts in the literature have been concentrated in designing zone abstraction operators that are exact in the sense that they preserve the reachability relation between the locations of a timed automaton; see [6]. The idea is to determine bounds on the constants to which a given clock can be compared to in a given part of the automaton, since the clock values do not matter outside these bounds. In [21,22], the authors give an algorithm where these bounds are dynamically adapted during the exploration, which allows one to obtain coarser abstractions. In [29], the exploration tree contains pairs of zones: a concrete zone as in the usual algorithm, and a coarser abstract zone. The algorithm explores all branches using the coarser zone and immediately refines the abstract zone whenever an edge which is disabled in the concrete zone is enabled. In [17], a CEGAR loop was used to solve timed games by analyzing strategies computed for each abstract game. The abstraction consisted in collapsing locations.

Some works have adapted the abstraction-refinement paradigm to timed automata. In [14], the authors apply "localization reduction" to timed automata within an abstraction-refinement loop: they abstract away clocks and discrete variables, and only introduce them as they are needed to rule out spurious counterexamples. A more general but similar approach was developed in [18]. In [31], the authors adapt the trace abstraction refinement idea to timed automata where a finite automaton is maintained to rule out infeasible edge sequences.

The CEGAR approach was also used recently in the LinAIG framework for verifying linear hybrid automata [1]. In this work, the backward reachability algorithm exploits *don't-cares* to reduce the size of the Boolean circuits representing the state space. The abstractions consist in enlarging the size of *don't-cares* to reduce the number of linear predicates used in the representation.

2 Timed Automata and Zones

2.1 Timed Automata

Given a finite set of clocks $\mathcal{C}$, we call *valuations* the elements of $\mathbb{R}^{\mathcal{C}}_{\geq 0}$. For a clock valuation v, a subset $R \subseteq \mathcal{C}$, and a non-negative real d, we denote with $v[R \leftarrow d]$ the valuation w such that $w(x) = v(x)$ for $x \in \mathcal{C} \setminus R$ and $w(x) = d$ for $x \in R$, and with $v + d$ the valuation w' such that $w'(x) = v(x) + d$ for all $x \in \mathcal{C}$. We extend these operations to sets of valuations in the obvious way. We write $\mathbf{0}$ for the valuation that assigns 0 to every clock. An *atomic guard* is a formula of

the form $x \prec k$ or $x - y \prec k$ with $x, y \in \mathcal{C}$, $k \in \mathbb{N}$, and $\prec \in \{<, \leq, >, \geq\}$. A *guard* is a conjunction of atomic guards. A valuation v satisfies a guard g, denoted $v \models g$, if all atomic guards hold true when each $x \in \mathcal{C}$ is replaced with $v(x)$. Let $[\![g]\!] = \{v \in \mathbb{R}^{\mathcal{C}}_{\geq 0} \mid v \models g\}$ denote the set of valuations satisfying g. We write $\Phi_{\mathcal{C}}$ for the set of guards built on $\mathcal{C}$.

A *timed automaton* $\mathcal{A}$ is a tuple $(\mathcal{L}, \mathsf{Inv}, \ell_0, \mathcal{C}, E)$, where $\mathcal{L}$ is a finite set of locations, $\mathsf{Inv}\colon \mathcal{L} \to \Phi_{\mathcal{C}}$ defines location invariants, $\mathcal{C}$ is a finite set of clocks, $E \subseteq \mathcal{L} \times \Phi_{\mathcal{C}} \times 2^{\mathcal{C}} \times \mathcal{L}$ is a set of edges, and $\ell_0 \in \mathcal{L}$ is the initial location. An edge $e = (\ell, g, R, \ell')$ is also written as $\ell \xrightarrow{g,R} \ell'$. For any location ℓ, we let $E(\ell)$ denote the set of edges leaving ℓ.

A *configuration* of $\mathcal{A}$ is a pair $q = (\ell, v) \in \mathcal{L} \times \mathbb{R}^{\mathcal{C}}_{\geq 0}$ such that $v \models \mathsf{Inv}(\ell)$. A *run* of $\mathcal{A}$ is a sequence $q_1 e_1 q_2 e_2 \ldots q_n$ where for all $i \geq 1$, $q_i = (\ell_i, v_i)$ is a configuration, and either $e_i \in \mathbb{R}_{>0}$, in which case $q_{i+1} = (\ell_i, v_i + e_i)$, or $e_i = (\ell_i, g_i, R_i, \ell_{i+1}) \in E$, in which case $v_i \models g_i$ and $q_{i+1} = (\ell_{i+1}, v_i[R_i \leftarrow 0])$. A *path* is a sequence of edges with matching endpoint locations.

2.2 Zones and DBMs

Several tools for timed automata implement algorithms based on *zones*, which are particular polyhedra definable with clock constraints. Formally, a zone Z is a subset of $\mathbb{R}^{\mathcal{C}}_{\geq 0}$ definable by a guard in $\Phi_{\mathcal{C}}$.

We recall a few basic operations defined on zones. First, the intersection $Z \cap Z'$ of two zones Z and Z' is clearly a zone. Given a zone Z, the set of time-successors of Z, defined as $Z\uparrow = \{v + t \in \mathbb{R}^{\mathcal{C}}_{\geq 0} \mid t \in \mathbb{R}_{\geq 0},\ v \in Z\}$, is easily seen to be a zone; similarly for time-predecessors $Z\downarrow = \{v \in \mathbb{R}^{\mathcal{C}}_{\geq 0} \mid \exists t \geq 0.\ v + t \in Z\}$. Given $R \subseteq \mathcal{C}$, we let $\mathsf{Reset}_R(Z)$ be the zone $\{v[R \leftarrow 0] \in \mathbb{R}^{\mathcal{C}}_{\geq 0} \mid v \in Z\}$, and $\mathsf{Free}_x(Z) = \{v' \in \mathbb{R}^{\mathcal{C}}_{\geq 0} \mid \exists v \in Z, d \in \mathbb{R}_{\geq 0}, v' = v[x \leftarrow d]\}$.

Zones can be represented as *difference-bound matrices (DBM)* [8,15]. Let $\mathcal{C}_0 = \mathcal{C} \cup \{0\}$, where 0 is an extra symbol representing a special clock variable whose value is always 0. A DBM is a $|\mathcal{C}_0| \times |\mathcal{C}_0|$-matrix taking values in $(\mathbb{Z} \times \{<, \leq\}) \cup \{(+\infty, <)\}$. Intuitively, cell (x, y) of a DBM M stores a pair $(d, \prec)$ representing an upper bound on the difference $x - y$. For any DBM M, we let $[\![M]\!]$ denote the zone it defines.

While several DBMs can represent the same zone, each zone admits a *canonical* representation, which is obtained by storing the tightest clock constraints defining the zone. This canonical representation can be obtained by computing shortest paths in a graph where the vertices are clocks and the edges weighted by clock constraints, with natural addition and comparison of elements of $(\mathbb{Z} \times \{<, \leq\}) \cup \{(+\infty, <)\}$. This graph has a negative cycle if, and only if, the associated DBM represents the empty zone.

All the operations on zones can be performed efficiently (in $O(|\mathcal{C}_0|^3)$) on their associated DBMs while maintaining reduced form. For instance, the intersection $N = Z \cap Z'$ of two canonical DBMs Z and Z' can be obtained by first computing the DBM $M = \min(Z, Z')$ such that $M(x, y) = \min\{Z(x, y), Z'(x, y)\}$ for all $(x, y) \in {\mathcal{C}_0}^2$, and then turning M into canonical form. We refer to [8] for

full details. By a slight abuse of notation, we use the same notations for DBMs as for zones, writing e.g. $M' = M\uparrow$, where M and M' are reduced DBMs such that $[\![M']\!] = [\![M]\!]\uparrow$. Given an edge $e = (\ell, g, R, \ell')$, and a zone Z, we define $\mathsf{Post}_e(Z) = \mathsf{Inv}(\ell') \cap (g \cap \mathsf{Reset}_R(Z))\uparrow$, and $\mathsf{Pre}_e(Z) = (g \cap \mathsf{Free}_R(\mathsf{Inv}(\ell') \cap Z))\downarrow$. For a path $\rho = e_1 e_2 \dots e_n$, we define Post_ρ and Pre_ρ by iteratively applying Post_{e_i} and Pre_{e_i} respectively.

2.3 Clock-Predicate Abstraction and Interpolation

For all clocks x and y in $\mathcal{C}_0$, we consider a finite set $\mathcal{D}_{x,y} \subseteq \mathbb{N} \times \{\leq, <\}$, and gather these in a table $\mathcal{D} = (\mathcal{D}_{x,y})_{x,y \in \mathcal{C}_0}$. $\mathcal{D}$ is the *abstract domain* which restricts zones to be defined only using constraints of the form $x - y \prec k$ with $(k, \prec) \in \mathcal{D}_{x,y}$, as seen earlier. Let us call $\mathcal{D}$ the *concrete domain* if $\mathcal{D}_{x,y} = \mathbb{N} \times \{\leq, <\}$ for all $x, y \in \mathcal{C}_0$. A zone Z is $\mathcal{D}$-definable if there exists a DBM D such that $Z = [\![D]\!]$ and $D(x,y) \in \mathcal{D}_{x,y}$ for all $x, y \in \mathcal{C}_0$. Note that we do not require this witness DBM D to be reduced; the reduction of such a DBM might introduce additional values. We say that domain $\mathcal{D}'$ is a *refinement* of $\mathcal{D}$ if for all $x, y \in \mathcal{C}_0$, we have $\mathcal{D}_{x,y} \subseteq \mathcal{D}'_{x,y}$.

An abstract domain $\mathcal{D}$ induces an *abstraction function* $\alpha_{\mathcal{D}} \colon 2^{\mathbb{R}^{\mathcal{C}}_{\geq 0}} \to 2^{\mathbb{R}^{\mathcal{C}}_{\geq 0}}$ where $\alpha_{\mathcal{D}}(Z)$ is the smallest $\mathcal{D}$-definable zone containing Z. For any reduced DBM D, $\alpha_{\mathcal{D}}([\![D]\!])$ can be computed by setting $D'(x,y) = \min\{(k, \prec) \in \mathcal{D}_{x,y} \mid D(x,y) \leq (k, \prec)\}$ (with $\min \emptyset = (\infty, <)$).

An *interpolant* for a pair of zones (Z_1, Z_2) with $Z_1 \cap Z_2 = \emptyset$ is a zone Z_3 with $Z_1 \subseteq Z_3$ and $Z_3 \cap Z_2 = \emptyset$[1] [29]. We use interpolants to refine our abstractions; in order not to add too many new constraints when refining, our aim is to find *minimal interpolants*: define the density of a DBM D as $d(D) = \#\{(x,y) \in {\mathcal{C}_0}^2 \mid D(x,y) \neq (\infty, <)\}$. Notice that while any pair of disjoint convex polyhedra can be separated by hyperplanes, not all pairs of disjoint zones admit interpolants of density 1; this is because not all (half-spaces delimited by) hyperplanes are zones. Still, we can bound the density of a minimal interpolant:

Lemma 1. *For any pair of disjoint, non-empty zones (A, B), there exists an interpolant of density less than or equal to $|\mathcal{C}_0|/2$.*

By adapting the algorithm of [29] for computing interpolants, we can compute minimal interpolants efficiently:

Proposition 2. *Computing a minimal interpolant can be performed in $O(|\mathcal{C}|^4)$.*

3 Enumerative Algorithm

The first type of algorithm we present is a zone-based enumerative algorithm based on the clock-predicate abstractions. Let us first describe the overall

[1] It is sometimes also required that the interpolant only involves clocks that have non-trivial constraints in both Z_1 and Z_2. We do not impose this requirement in our definition, but it will hold true in the interpolants computed by our algorithm.

algorithm in Algorithm 1, which is a typical abstraction-refinement loop. We then explain how the abstract reachability and refinement procedures are instantiated.

Algorithm 1. Enumerative algorithm checking the reachability of a target location ℓ_T.

```
   Input: A = (L, lnv, ℓ0, C, E), ℓT
1  Initialize D0;
2  wait:= {node(ℓ0, 0↑, D0)};
3  passed:= ∅;
4  while do
5      π := AbsReach(A, wait,
         passed, ℓT);
6      if π = ∅ then
7          return Not reachable;
8      else
9          if trace π is feasible then
10             return Reachable;
11         else
               Refine(π, wait, passed);
12 return Not reachable;
```

Algorithm 2. AbsReach

```
   Input: (L, lnv, l0, C, E), wait, passed,
          ℓT
1  while wait ≠ ∅ do
2      n := wait.pop();
3      if n.ℓ = ℓT then
4          return Trace from root to n;
5      if ∃n' ∈ passed such that n.ℓ =
         n'.ℓ ∧ n.Z ⊆ n'.Z then
6          n.covered := n';
7      else
8          n.Z := α(n.Z, n);
9          passed.add(n);
10         for e = (ℓ, g, R, ℓ') ∈ E(n.ℓ)
             s.t. Z' := Post_e(n.Z) ≠ ∅
             do
11             D' := choose-dom(n, e);
12             n' := node(ℓ', Z', D');
13             n'.parent := n;
14             wait.add(n');
15 return ∅;
```

The initialization at line 1 chooses an abstract domain for the initial state, which can be either empty (thus the coarsest abstraction) or defined according to some heuristics. The algorithm maintains the wait and passed lists that are used in the forward exploration. As usual, the wait list can be implemented as a stack, a queue, or another priority list that determines the search order. The algorithm also uses covering nodes. Indeed if there are two node n and n', with $n \in$ passed, $n' \in$ wait, $n.\ell = n'.\ell$, and $n'.z \subseteq n.Z$, then we know that every location reachable from n' is also reachable from n. Since we have already explored n and we generated its successors, there is no need to explore the successors of n'. The algorithm explicitly creates an exploration tree: line 2 creates a node containing location ℓ_0, zone $\mathbf{0}\uparrow$, and the abstract domain $\mathcal{D}_0$ as the root of our tree, and adds this to the wait list. More details on the tree are given in the next subsection. Procedure AbsReach then looks for a trace to the target location ℓ_T. If such a trace exists, line 9 checks its feasibility. Here π is a sequence of node and edges of $\mathcal{A}$. The feasibility check is done by computing predecessors with zones starting from the final state, without using the abstraction function. If the last zone intersects our initial zone, this means that the trace is feasible. More details are given in Sect. 3.2.

3.1 Abstract Forward Reachability: AbsReach

We give a generic algorithm independently from the implementations of the abstraction functions and the refinement procedure.

Algorithm 2 describes the reachability procedure under a given abstract domain $\mathcal{D}$. It is similar to the standard forward reachability algorithm using a wait-list and a passed-list. We explicitly create an exploration tree where the leaves are nodes in wait, covered nodes, or nodes that have no non-empty successors. Each node n contains the fields ℓ, Z which are labels describing the current location and zone; field covered points to a node covering the current node (it is undefined if the current node is not (known to be) covered); field parent points to the parent node in the tree (it is undefined for the root); and field $\mathcal{D}$ is the abstract domain associated with the node. Thus, the algorithm uses a possibly different abstract domain for each node in the exploration tree.

The difference of our algorithm w.r.t. the standard reachability can be seen at lines 8 and 11. At line 8, we apply the abstraction function to the zone taken from the wait-list before adding it to the passed-list. The abstraction function α is a function of a zone Z and a node n. This allows one to define variants with different dependencies; for instance, α might depend on the abstract domain $n.\mathcal{D}$ at the current node, but it can also use other information available in n or on the path ending in n. For now, it is best to think of α simply as $Z \mapsto \alpha_{n.\mathcal{D}}(Z)$. At line 11, the function choose-dom chooses an abstract domain for the node n'. The domain could be chosen global for all nodes, or local to each node. A good trade-off, which we used in our experiments, is to have domains associated with locations of the timed automaton.

Remark 1. Note that we use the abstraction function when the node is inserted in the passed list. This is because we want the node to contain the smallest zone possible when we test whether the node is covered. We only need to use the abstracted zone when we compute its successor and when we test whether the node is covering. This allows us to store a unique zone.

As a first step towards proving correctness of our algorithm, we show that the following property is preserved by Algorithm AbsReach:

> For all nodes n in passed, for all edges e from $n.\ell$, if $\mathsf{Post}_e(n.Z) \neq \emptyset$, then n has a child n' such that $\mathsf{Post}_e(n.Z) \subseteq n'.Z$. If n' is in passed, then we also have $\alpha_{n'.\mathcal{D}}(\mathsf{Post}_e(n.Z)) \subseteq n'.Z$. (1)

Lemma 3. *Algorithm* AbsReach *preserves Property* (1).

Note that although we use inclusion in Property (1), AbsReach would actually preserve equality of zones, but we will not always have equality before running AbsReach. This is because Refine might change the zones of some nodes without updating the zones of all their descendants.

3.2 Refinement: Refine

We now describe our refinement procedure Refine. Let us now assume that AbsReach returns $\pi = A_1 \xrightarrow{\sigma_1} A_2 \xrightarrow{\sigma_2} \dots \xrightarrow{\sigma_{k-1}} A_k$, and write $\mathcal{D}_i$ for the domain associated with each A_i. We write C_1 for the initial concrete zone, and for $i < k$, we define $C_{i+1} = \mathsf{Post}_{\sigma_i}(A_i)$. We also note $Z_k = A_k$ and for $i < k$, $Z_i = \mathsf{Pre}_{\sigma_i}(Z_{i+1}) \cap A_i$. Then π is not feasible if, and only if, $\mathsf{Post}_{\sigma_1 \dots \sigma_k}(C_1) = \emptyset$, or equivalently $\mathsf{Pre}_{\sigma_1 \dots \sigma_k}(A_k) \cap C_1 = \emptyset$. Since for all $i < k$, it holds $C_i \subseteq A_{i+1}$, we have that π is not feasible if, and only if, $\exists i \leq k.\ C_i \cap Z_i = \emptyset$. We illustrate this on Fig. 2.

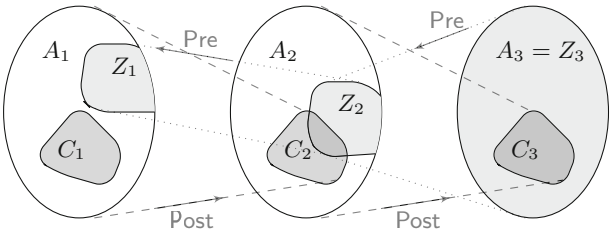


Fig. 2. Spurious counter-example: $Z_1 \cap C_1 = \emptyset$

Let us assume that π is not feasible. Let us denote by i_0 the maximal index such that $C_{i_0} \cap Z_{i_0} = \emptyset$. This index also has the property that for all $j < i_0$, we have $Z_j = \emptyset$ and $Z_{i_0} \neq \emptyset$. Once we have identified this trace as spurious by computing the Z_j, we have two possibilities:

- if $Z_{i_0} \cap \alpha_{\mathcal{D}_{i_0}}(C_{i_0}) \neq \emptyset$: this means that we can reach A_k from $\alpha_{\mathcal{D}_{i_0}}(C_{i_0})$ but not from C_{i_0}. In other words, our abstraction is too coarse and we must add some values to $\mathcal{D}_{i_0}$ so that $Z_{i_0} \cap \alpha_{\mathcal{D}_{i_0}}(C_{i_0}) = \emptyset$. Those values are found by computing the interpolant of Z_{i_0} and C_{i_0}
- Otherwise it means that $\alpha_{\mathcal{D}_{i_0}}(C_{i_0})$ cannot reach A_k and the only reason the trace exists is because either $\mathcal{D}_{i_0}$ or A_{i_0-1} has been modified at some point and A_{i_0} was not modified accordingly.

We can then update the values of C_i for $i > i_0$ and repeat the process until we reach an index j_0 such that $C_{j_0} = \emptyset$. We then have modified the nodes $n_{i_0}, \dots, n_{j_0}$ and knowing that $n_{j_0}.Z = \emptyset$, we can delete it and all of its descendants. Since some of the descendants of n_{i_0} have not been modified, this might cause some refinements of the first type in the future. In order to ensure termination, we sometimes have to cut a subtree from a node in $n_{i_0}, \dots, n_{j_0-1}$ and reinsert it in the wait list to restart the exploration from there. We call this action cut, and we can use several heuristics to decide when to use it. In the rest of this paper we will use the following heuristics: we perform cut on the first node of $n_{i_0} \dots n_{j_0}$ that is covered by some other node. Since this node is covered, we know that we will not restart the exploration from this node, or that the

node was covered by one of its descendant. If none of these nodes are covered, we delete n_{j_0} and its descendants. Other heuristics are possible, for instance applying cut on n_{i_0}. We found that the above heuristics was the most efficient in our experiments.

Lemma 4. *Pick a node n, and let $Y = n.Z$. Then after running* Refine*, either node n is deleted, or it holds $n.Z \subseteq Y$. In other words, the zone of a node can only be reduced by* Refine*.*

It follows that Refine also preserves Property (1), so that:

Lemma 5. *Algorithm 1 satisfies Property* (1)*.*

We can then prove that our algorithm correctly decides the reachability problem and always terminates.

Theorem 6. *Algorithm 1 terminates and is correct.*

4 Symbolic Algorithm

4.1 Boolean Encoding of Zones

We now present a symbolic algorithm that represents abstract states using Boolean formulas. Let $\mathbb{B} = \{0, 1\}$, and $\mathcal{V}$ be a set of variables. A Boolean formula f that uses variables from set $X \subseteq \mathcal{V}$ will be written $f(X)$ to make the dependency explicit; we sometimes write $f(X, Y)$ in place of $f(X \cup Y)$. Such a formula represents a set $[\![f]\!] = \{v \in \mathbb{B}^{\mathcal{V}} \mid v \models f\}$. We consider primed versions of all variables; this will allow us to write formulas relating two valuations. For any subset $X \subseteq \mathcal{V}$, we define $X' = \{p' \mid p \in X\}$.

A *literal* is either p or $\neg p$ for a variable p. Given a set X of variables, an *X-minterm* is the conjunction of literals where each variable of X appears exactly once. X-minterms can be seen as elements of $\mathbb{B}^X$. Given a vector of Boolean formulas $Y = (Y_x)_{x \in X}$, formula $f[Y/X]$ is the *substitution of X by Y in f*, obtained by replacing each $x \in X$ with the formula Y_x. The positive cofactor of $f(X)$ by x is $\exists x.\ (x \wedge f(X))$, and its negative cofactor is $\exists x.\ (\neg x \wedge f(X))$.

Let us define a generic operator `post` that computes successors of a set $S(X, Y)$ given a relation $R(X, X')$ (here, Y designates any set of variables on which S might depend outside of X): $\texttt{post}_R(S(X, Y)) = (\exists X.S(X, Y) \wedge R(X, X'))[X/X']$. Similarly, we set $\texttt{pre}_R(S(X, Y)) = (\exists X'.S(X, Y)[X'/X] \wedge R(X, X'))$, which computes the predecessors of $S(X, Y)$ by the relation R [24].

Clock Predicate Abstraction. We fix a total order $\lhd$ on $\mathcal{C}_0$. In this section, abstract domains are defined as $\mathcal{D} = (\mathcal{D}_{x,y})_{x \lhd y \in \mathcal{C}_0}$, that is only for pairs $x \lhd y$. In fact, constraints of the form $x - y \leq k$ with $x \rhd y$ are encoded using the negation of $y - x < -k$ since $(x - y \leq k) \Leftrightarrow \neg(y - x < -k)$. We thus define $\mathcal{D}_{x,y} = -\mathcal{D}_{y,x}$ for all $x \rhd y$.

For $x, y \in \mathcal{C}_0$, let $\mathcal{P}_{x,y}$ denote the set of *clock predicates associated to* $\mathcal{D}_{x,y}$:

$$\mathcal{P}^{\mathcal{D}}_{x,y} = \{P_{x-y\prec k} \mid (k, \prec) \in \mathcal{D}_{x,y}\}.$$

Let $\mathcal{P}^{\mathcal{D}} = \cup_{x,y\in\mathcal{C}_0}\mathcal{P}_{x,y}$ denote the set of all clock predicates associated with $\mathcal{D}$ (we may omit the superscript $\mathcal{D}$ when it is clear). For all $(x, y) \in {\mathcal{C}_0}^2$ and $(k, \prec) \in \mathcal{D}_{x,y}$, we denote by $p_{x-y\prec k}$ the literal $P_{x-y\prec k}$ if $x \lhd y$, and $\neg P_{y-x\prec^{-1}-k}$ otherwise (where $\leq^{-1} = <$ and $<^{-1} = \leq$). We also consider a set $\mathcal{B}$ of Boolean variables used to encode locations. Overall, the state space is described using Boolean formulas on these two types of variables, so states are elements of $\mathbb{B}^{\mathcal{P}\cup\mathcal{B}}$.

Our Boolean encoding of clock constraints and semantic operations follow those of [28] for a concrete domain. We define these however for abstract domains, and show how successor computation and refinement operations can be performed.

Let us define the *clock semantics* of predicate $P_{x-y\preceq k}$ as $[\![P_{x-y\preceq k}]\!]_{\mathcal{C}_0} = \{\nu \in \mathbb{R}^{\mathcal{C}_0}_{\geq 0} \mid \nu(x) - \nu(y) \preceq k\}$. Since the set $\mathcal{C}$ of clocks is fixed, we may omit the subscript and just write $[\![P_{x-y\preceq k}]\!]$. We define the conjunction, disjunction, and negation as intersection, union, and complement, respectively. Given a $\mathcal{P}$-minterm $v \in \mathbb{B}^{\mathcal{P}}$, we define $[\![v]\!]_{\mathcal{D}} = \bigcap_{p \text{ s.t. } v(p)}[\![p]\!]_{\mathcal{D}} \cap \bigcap_{p \text{ s.t. } \neg v(p)}[\![p]\!]^{c}_{\mathcal{D}}$. Thus, negation of a predicate encodes its complement. For a Boolean formula $F(\mathcal{P})$, we set $[\![F]\!] = \bigcup_{v\in\mathsf{Minterms}(F)}[\![v]\!]_{\mathcal{D}}$. Intuitively, the minterms of $\mathcal{P}$ define smallest zones of $\mathbb{R}^{\mathcal{C}}_{\geq 0}$ definable using $\mathcal{P}$. A minterm $v \in \mathbb{B}^{\mathcal{B}\cup\mathcal{P}}$ defines a pair $[\![v]\!]_{\mathcal{D}} = (l, Z)$ where l is encoded by $v_{|\mathcal{B}}$ and $Z = [\![v_{|\mathcal{P}}]\!]_{\mathcal{D}}$. A Boolean formula F on $\mathcal{B} \cup \mathcal{P}$ defines a set $[\![F]\!]_{\mathcal{D}} = \cup_{v\in\mathsf{Minterms}(F)}[\![v]\!]_{\mathcal{D}}$ of such pairs. A minterm v is *satisfiable* if $[\![v]\!]_{\mathcal{D}} \neq \emptyset$.

An abstract domain $\mathcal{D}$ induces an *abstraction function* $\alpha_{\mathcal{D}} \colon 2^{\mathbb{R}^{\mathcal{C}}_{\geq 0}} \to 2^{\mathbb{B}^{\mathcal{P}}}$ with $\alpha_{\mathcal{D}}(Z) = \{v \mid v \in \mathbb{B}^{\mathcal{P}} \text{ and } [\![v]\!]_{\mathcal{D}} \cap Z \neq \emptyset\}$, from the set of zones to the set of subsets of Boolean valuations on $\mathcal{P}$. We define the *concretization function* as $[\![\cdot]\!]_{\mathcal{D}} \colon 2^{\mathbb{B}^{\mathcal{P}}} \to 2^{\mathbb{R}^{\mathcal{C}}_{\geq 0}}$. The pair $(\alpha_{\mathcal{D}}, [\![\cdot]\!]_{\mathcal{D}})$ is a Galois connection, and $[\![\alpha_{\mathcal{D}}(Z)]\!]_{\mathcal{D}}$ is the most precise abstraction of Z in the domain induced by $\mathcal{D}$. Notice that $\alpha_{\mathcal{D}}$ is non-convex in general: for instance, if the clock predicates are $x \leq 2, y \leq 2$, then the set defined by the constraint $x = y$ maps to $(p_{x\leq 2} \wedge p_{y\leq 2}) \vee (\neg p_{x\leq 2} \wedge \neg p_{y\leq 2})$.

4.2 Reduction and Successor Computation

We now define the reduction operation, which is similar to the reduction of DBMs. The idea is to eliminate unsatisfiable minterms from a given Boolean formula. For example, we would like to make sure that in all minterms, if $p_{x-y\leq 1}$ holds, then so does $p_{x-y\leq 2}$, when both are available predicates. Another issue is to eliminate minterms that are unsatisfiable due to triangle inequality. This is similar to the shortest path computation used to turn DBMs in canonical form.

Example 1. Given predicates $\mathcal{P} = \{p_{x-y\leq 1}, p_{y-z\leq 1}, p_{x-z\leq 2}\}$, the formula $p_{x-y\leq 1} \wedge p_{y-z\leq 1}$ is not reduced since it contains the unsatisfiable minterm

$p_{x-y\leq 1} \wedge p_{y-z\leq 1} \wedge \neg p_{x-z\leq 2}$. However, the same formula is reduced if $\mathcal{P} = \{p_{x-y\leq 1}, p_{y-z\leq 1}\}$.

In this paper, we use limited reduction, since reductions are the most expensive operations in our algorithms. The following formula corresponds to 2-reduction, which intuitively amounts to applying shortest paths for paths of lengths 1 and 2:

$$\bigwedge_{\substack{(x,y)\in\mathcal{C}_0{}^2\\(k,\prec)\in\mathcal{D}_{x,y}}} \left[p_{x-y\prec k} \leftarrow \Big(\bigvee_{\substack{(l_1,\prec_1)\in\mathcal{D}_{x,y}\\(l_1,\prec_1)\leq(k,\prec)}} p_{x-y\prec_1 l_1} \vee \bigvee_{\substack{z\in\mathcal{C}_0,(l_1,\prec_1)\in\mathcal{D}_{x,z},\\(l_2,\prec_2)\in\mathcal{D}_{z,y}\\(l_1,\prec_1)+(l_2,\prec_2)\leq(k,\prec)}} p_{x-z\prec l} \wedge p_{z-y\prec' l'} \Big) \right]$$

Lemma 7. *For all formulas $S(\mathcal{P})$, we have $[\![S]\!]_{\mathcal{D}} = [\![\mathsf{reduce}^2_{\mathcal{D}}(S)]\!]_{\mathcal{D}}$ and all minterms of $\mathsf{reduce}^2_{\mathcal{D}}(S)$ are 2-reduced.*

Since 2-reduction des not consider shortest paths of all lengths, there are, in general, 2-reduced unsatisfiable minterms. Nevertheless, any abstraction can be refined so that the updated 2-reduction eliminates a given unsatisfiable minterm:

Lemma 8. *Let $v \in \mathbb{B}^{\mathcal{P}^{\mathcal{D}}}$ be a minterm such that $v \models \mathsf{reduce}^2_{\mathcal{D}}$ and $[\![v]\!] = \emptyset$. One can compute in polynomial time a refinement $\mathcal{D}' \supset \mathcal{D}$ such that $v \not\models \mathsf{reduce}^2_{\mathcal{D}'}$.*

We now explain how successor computation is realized in our encoding. For a guard g, assume we have computed an abstraction $\alpha_{\mathcal{D}}(g)$ in the present abstract domain. For each transition $\sigma = (\ell_1, g, R, \ell_2)$, let us define the formula $T_\sigma = \ell_1 \wedge \alpha_{\mathcal{D}}(g)$. We show how each basic operation on zones can be computed in our BDD encoding. In our algorithm, all formulas $A(\mathcal{B}, \mathcal{P})$ representing sets of states are assumed to be reduced, that is, $A(\mathcal{B}, \mathcal{P}) \subseteq \mathsf{reduce}^2_{\mathcal{D}}(A(\mathcal{B}, \mathcal{P}))$.

The intersection operation is simply logical conjunction:

Lemma 9. *For all reduced formulas $A(\mathcal{P})$ and $B(\mathcal{P})$, we have $A(\mathcal{P}) \wedge B(\mathcal{P}) = \alpha_{\mathcal{D}}([\![A(\mathcal{P})]\!]_{\mathcal{D}} \cap [\![B(\mathcal{P})]\!]_{\mathcal{D}})$.*

For the time successors, we define $\mathsf{Up}(A(\mathcal{B}, \mathcal{P})) = \mathsf{reduce}(\mathtt{post}_{S_{\mathsf{Up}}}(A(\mathcal{B}, \mathcal{P})))$ where

$$S_{\mathsf{Up}} = \bigwedge_{\substack{x\in\mathcal{C}\\(k,\prec)\in\mathcal{D}_{x,0}}} (\neg p_{x-0\prec k} \rightarrow \neg p'_{x-0\prec k}) \bigwedge_{\substack{x,y\in\mathcal{C}_0,x\neq 0\\(k,\prec)\in\mathcal{D}_{x,y}}} (p'_{x-y\prec k} \leftrightarrow p_{x-y\prec k}).$$

Lemma 10. *For any Boolean formula $A(\mathcal{B}, \mathcal{P})$, $\alpha_{\mathcal{D}}([\![A]\!]\uparrow) \subseteq \mathsf{Up}(A)$. Moreover, if $\mathcal{D}$ is the concrete domain and A is reduced, then this holds with equality.*

Following similar ideas, we handle clock resets by defining $\mathsf{Reset}_z(A) = \mathsf{reduce}(\mathtt{post}_{S_{\mathsf{Reset}_z}}(A))$, for a (complex) relation S_{Reset_z} to encode how predicates evolve (see the long version [27] of this article for more detailled explanations).

We get:

Lemma 11. *For any Boolean formula $A(\mathcal{B}, \mathcal{P})$, and any clock $z \in \mathcal{C}$, we have $\alpha_{\mathcal{D}}(\mathtt{Reset}_z([\![A]\!]_{\mathcal{D}})) \subseteq \mathsf{Reset}_z(A)$. Moreover, if $\mathcal{D}$ is the concrete domain, and A is reduced, then the above holds with equality.*

Algorithm 3. Algorithm SymReach that checks the reachability of a target location l_T in a given abstract domain $\mathcal{D}$.

Input: $\mathcal{A} = (\mathcal{L}, \mathsf{Inv}, \ell_0, \mathcal{C}, E)$, ℓ_T, $\mathcal{D}$

```
1  ;
2  next := enc(l_0) ∧ α_D(∧_{x∈C} x = 0);
3  layers := [];
4  reachable := false;
5  while (¬reachable ∧ next) ≠ false do
6  |   reachable := reachable ∨ next;
7  |   next := ApplyEdges(Up(next)) ∧ ¬reachable;
8  |   layers.push(next);
9  |   if (next ∧ enc(l_T)) ≠ false then
10 |   |   return ExtractTrace (layers);
11 return Not reachable;
```

4.3 Model-Checking Algorithm

Algorithm 3 shows how to check the reachability of a target location given an abstract domain. The list layers contains, at position i, the set of states that are reachable in i steps. The function ApplyEdges computes the disjunction of immediate successors by all edges. It consists in looping over all edges $e = (l_1, g, R, l_2)$, and gathering the following image by e:

$$\mathsf{enc}(\ell_2) \wedge \mathsf{Reset}_{r_k}(\mathsf{Reset}_{r_{k-1}}(\ldots(\mathsf{Reset}_{r_1}((((\exists \mathcal{B}.A(\mathcal{B},\mathcal{P}) \wedge \mathsf{enc}(\ell_1)) \wedge \alpha_{\mathcal{D}}(g)))))))),$$

where $R = \{r_1, \ldots, r_k\}$. We thus use a partitioned transition relation and do not compute the monolithic transition relation.

When the target location is found to be reachable, ExtractTrace(layers) returns a trace reaching the target location. This is standard and can be done by computing backwards from the last element of layers, by finding which edge can be applied to reach the current state. Since both reset and time successor operations are defined using relations, predecessors in our abstract system can be easily computed using the operator $\mathtt{pre}_R$. As it is standard, we omit the precise definition of this function (the reader can refer to the implementation) but assume that it returns a trace of the form $A_1 \xrightarrow{\sigma_1} A_2 \xrightarrow{\sigma_2} \ldots \xrightarrow{\sigma_{n-1}} A_n$, where the $A_i(\mathcal{B},\mathcal{P})$ are minterms and the σ_i belong to the trace alphabet $\Sigma = \{\mathrm{up}, r_\emptyset\} \cup \{r(x)\}_{x\in\mathcal{C}}$, with the following meaning:

- if $A_i \xrightarrow{\mathrm{up}} A_{i+1}$ then $A_{i+1} = \mathsf{Up}(A_i)$;
- if $A_i \xrightarrow{r_\emptyset} A_{i+1}$ then $A_{i+1} = A_i$;
- if $A_i \xrightarrow{r(x)} A_{i+1}$ then $A_{i+1} = \mathsf{Reset}_x(A_i)$.

The feasibility of such a trace is easily checked using DBMs.

The overall algorithm then follows a classical CEGAR scheme. We initialize $\mathcal{D}$ by adding the clock constraints that appear syntactically in $\mathcal{A}$, which is often

a good heuristic. We run the reachability check of Algorithm 3. If no trace is found, then the target location is not reachable. If a trace is found, then we check for feasibility. If it is feasible, then the counterexample is confirmed. Otherwise, the trace is spurious and we run the refinement procedure described in the next subsection, and repeat the analysis.

4.4 Abstraction Refinement

Since we initialize $\mathcal{D}$ with all clock constraints appearing in guards, we can assume that all guards are represented exactly in the considered abstractions. Note that the algorithm can be easily extended to the general case; but this simplifies the presentation.

The abstract transition relation we use is not the most precise abstraction of the concrete transition relation. Therefore, it is possible to have abstract transitions $A_1 \xrightarrow{a} A_2$ for some action a while no concrete transition exists between $[\![A_1]\!]$ and $[\![A_2]\!]$. This requires care and is not a direct application of the standard refinement technique from [11]. A second difficulty is due to incomplete reduction of the predicates using $\mathsf{reduce}^2_{\mathcal{D}}$. In fact, some reachable states in our abstract model will be unsatisfiable. Let us explain how we refine the abstraction in each of these cases.

Consider an algorithm interp which returns an interpolant of given zones Z_1, Z_2. In what follows, by the *refinement of* $\mathcal{D}$ *by* $\mathsf{interp}(Z_1, Z_2)$, we mean the domain $\mathcal{D}'$ obtained by adding $(k, \prec)$ to $\mathcal{D}_{x,y}$ for all constraints $x - y \prec k$ of $\mathsf{interp}(Z_1, Z_2)$. Observe that $\alpha_{\mathcal{D}'}(Z_1) \cap \alpha_{\mathcal{D}'}(Z_2) = \emptyset$ in this case.

We define concrete successor and predecessor operations for the actions in Σ. For each $a \in \Sigma$, let Pre^c_a denote the concrete predecessor operation on zones defined straightforwardly, and similarly for Post^c_a.

Consider domain $\mathcal{D}$ and the induced abstraction function $\alpha_{\mathcal{D}}$. Assume that we are given a spurious trace $\pi = A_1 \xrightarrow{\sigma_1} A_2 \xrightarrow{\sigma_1} \dots \xrightarrow{\sigma_{n-1}} A_n$. Let $B_1 \dots B_n$ be the sequence of concrete states visited along π in $\mathcal{A}$, that is, B_1 is the concrete initial state, and for all $2 \leq i \leq n$, let $B_i = \mathsf{Post}^c_{\pi_{i-1}}(B_{i-1})$. This sequence can be computed using DBMs.

The trace is *realizable* if $B_n \neq \emptyset$, in which case the counterexample is confirmed. Otherwise it is *spurious*. We show how to refine the abstraction to eliminate a spurious trace π.

Let i_0 be the maximal index such that $B_{i_0} \neq \emptyset$. There are three possible reasons explaining why B_{i_0+1} is empty:

1. first, if the abstract successor A_{i_0+1} is unsatisfiable, that is, if it contains contradictory predicates; in this case, $[\![A_{i_0+1}]\!] = \emptyset$, and the abstraction is refined by Lemma 8 to eliminate this case by strengthening $\mathsf{reduce}^k_{\mathcal{D}}$.
2. if there are predecessors of A_{i_0+1} inside A_{i_0} but none of them are in B_{i_0}, i.e., $\mathsf{Pre}^c_{\pi_{i_0}}([\![A_{i_0+1}]\!]) \cap [\![A_{i_0}]\!] \neq \emptyset$; in this case, we refine the domain by separating these predecessors from the rest of A_{i_0} using $\mathsf{interp}(\mathsf{Pre}^c_{\pi_{i_0}}([\![A_{i_0+1}]\!]), B_{i_0-1})$, as in [11].

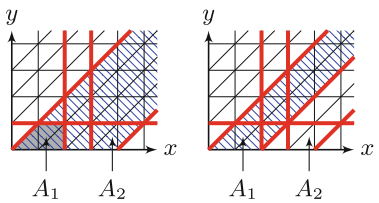
3. otherwise, there are no predecessors of A_{i_0+1} inside A_{i_0}: we refine the abstraction according to the type of the transition from step i_0 to i_0+1:
   (a) if $\pi_{i_0} = \text{up}$: refine $\mathcal{D}$ by $\mathsf{interp}([\![A_{i_0}]\!]\uparrow, [\![A_{i_0+1}]\!]\downarrow)$.
   (b) if $\pi_{i_0} = r(x)$: refine $\mathcal{D}$ by $\mathsf{interp}(\mathsf{Free}_x([\![A_{i_0}]\!]), \mathsf{Free}_x([\![A_{i_0+1}]\!]))$.

Note that the case $\pi_{i_0} = r_\emptyset$ is not possible since this induces the identity function both in the abstract and concrete systems.

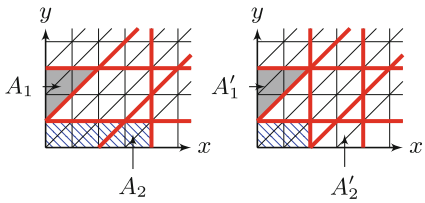
Given abstraction $\alpha_{\mathcal{D}}$ and spurious trace π, let $\mathsf{refine}(\alpha_{\mathcal{D}}, \pi)$ denote the refined abstraction $\alpha_{\mathcal{D}'}$ obtained as described above.

The following two lemmas justify the two subcases of the third case above. They prove that the detected spurious transition disappears after refinement. The reset and up operations depend on the abstraction, so we make this dependence explicit below by using superscripts, as in Reset_x^α and Up^α, in order to distinguish the operations before and after a refinement.

Lemma 12. *Consider* $(A_1, A_2) \in \mathsf{Up}^\alpha$ *with* $[\![A_1]\!]\uparrow \cap [\![A_2]\!] = \emptyset$. *Then* $[\![A_1]\!]\uparrow \cap [\![A_2]\!]\downarrow = \emptyset$. *Moreover, if* α' *is obtained by refinement of* α *by* $\mathsf{interp}([\![A_1]\!]\uparrow, [\![A_2]\!]\downarrow)$, *then for all* $(A_1', A_2') \in \mathsf{Up}^{\alpha'}$, $[\![A_1']\!] \subseteq [\![A_1]\!]$ *implies* $[\![A_2']\!] \cap [\![A_2]\!] = \emptyset$.



(a) Refinement for the time successors operation. The interpolant that separates $[\![A_1]\!]\uparrow$ from $[\![A_2]\!]\downarrow$ contains the constraint $x = y + 2$. When this is added to the abstract domain, the set A_2' (which is A_2 in the new abstraction) is no longer reachable by the time successors operation.



(b) Refinement for the reset operation. The interpolant that separates $\mathsf{Free}_y(A_1)$ from $\mathsf{Free}_y(A_2)$ contains the constraint $x < 2$. When this is added to the abstract domain, the set A_2' (which is A_2 in the new abstraction) is no longer reachable by the reset operation.

Lemma 13. *Consider* $x \in \mathcal{C}$, *and* $(A_1, A_2) \in \mathsf{Reset}_x^\alpha$ *such that* $[\![A_1]\!][x \leftarrow 0] \cap [\![A_2]\!] = \emptyset$. *Then* $\mathsf{Free}_x([\![A_1]\!]) \cap \mathsf{Free}_x([\![A_2]\!]) = \emptyset$. *Moreover, if* α' *is obtained by refinement of* α *by* $\mathsf{interp}(\mathsf{Free}_x([\![A_1]\!]), \mathsf{Free}_x([\![A_2]\!]))$, *then for all* $(A_1', A_2') \in \mathsf{Reset}_x^{\alpha'}$ *with* $[\![A_1']\!] \subseteq [\![A_1]\!]$, *we have* $[\![A_2']\!] \cap [\![A_2]\!] = \emptyset$.

5 Experiments

We implemented both algorithms. The symbolic version was implemented in OCaml using the CUDD library[2]; the explicit version was implemented in C++ within an existing model checker using Uppaal DBM library. Both prototypes

[2] http://vlsi.colorado.edu/~fabio/.

take as input networks of timed automata with invariants, discrete variables, urgent and committed locations. The presented algorithms are adapted to these features without difficulty.

We evaluated our algorithms on three classes of benchmarks we believe are significant. We compare the performance of the algorithm with that of Uppaal [7] which is based on zones, as well as the BDD-based model checker engine of PAT [25]. We were unable to compare with RED [30] which is not maintained anymore and not open source, and with which we failed to obtain correct results. The tool used in [16] was not available either. We thus only provide a comparison here with two well-maintained tools.

Two of our benchmarks are variants of schedulability-analysis problems where task execution times depend on the internal states of executed processes, so that an analysis of the state space is necessary to obtain a precise answer.

Monoprocess Scheduling Analysis. In this variant, a single process sequentially executes tasks on a single machine, and the execution time of each cycle depends on the state of the process. The goal is to determine a bound on the maximum execution time of a single cycle. This depends on the semantics of the process since the bound depends on the reachable states.

More precisely, we built a set of benchmarks where the processes are defined by synchronous circuit models taken from the Synthesis Competition (http://www.syntcomp.org). We assume that each latch of the circuit is associated with a resource, and changing the state of the resource takes some amount of time. So a subset of the latches have clocks associated with them, which measure the time elapsed since the latest value change (latest moment when the value changed from 0 to 1, or from 1 to 0). We provide two time positive bounds ℓ_0 and ℓ_1 for each latch, which determine the execution time as follows: if the value of latch ℓ changes from 0 to 1 (resp. from 1 to 0), then the execution time of the present cycle cannot be less than ℓ_1 (resp. ℓ_0). The execution time of the step is then the minimum that satisfies these constraints.

Multi-process Stateful Scheduling Analysis. In this variant, three processes are scheduled on two machines with a round-robin policy. Processes schedule tasks one after the other without any delay. As in the previous benchmarks, a process executing a task (on any machine) corresponds to a step of the synchronous circuit model. Each task is described by a tuple (C_1, C_2, D) which defines the minimum and maximum execution times, and the relative deadline. When a task finishes, the next task arrives immediately. The values in the tuple depend on the state of the process. The goal is to check the absence of any deadline miss. Processes are also instantiated with AIG circuits from http://www.syntcomp.org.

Asynchronous Computation. We consider an asynchronous network of "threshold gates", defined as follows: each gate is characterized by a tuple $(n, \theta, [l, u])$ where n is the number of inputs, $0 \leq \theta \leq n$ is the threshold, and $l \leq u$ are lower and upper bounds on activation time. Each gate has an output which is initially undefined. The gate becomes active during the time period $[l, u]$.

During this time, if all inputs are defined, and if at least θ of the inputs have value 1, then it sets its output to 1. At the end of the time period, it becomes deactivated and the output becomes undefined again, until the next period, which starts l time units after the deactivation. The goal is to check whether the given gate can output 1 within a given time bound T.

Results. Figure 3 displays the results of our experiments. All algorithms were given 8 GB of memory and a timeout of 30 min, and the experiments were run on laptop with an Intel i7@3.2 Ghz processor running Linux. The symbolic algorithm performs best among all on the monoprocess and multiprocess scheduling benchmarks. Uppaal is the second best, but does not solve as many benchmarks as our algorithm. Our enumerative algorithm quickly fails on these benchmarks, often running out of memory. On asynchronous computation benchmarks, our enumerative algorithm performs remarkably well, beating all other algorithms. We ran our tools on the CSMA/CD benchmarks (with 3 to 12 processes); Uppaal performs the best but our enumerative algorithm is slightly behind. The symbolic algorithm does not scale, while PAT fails to terminate in all cases.

The tool used for the symbolic algorithm is open source and can be found at https://github.com/osankur/symrob along with all the benchmarks.

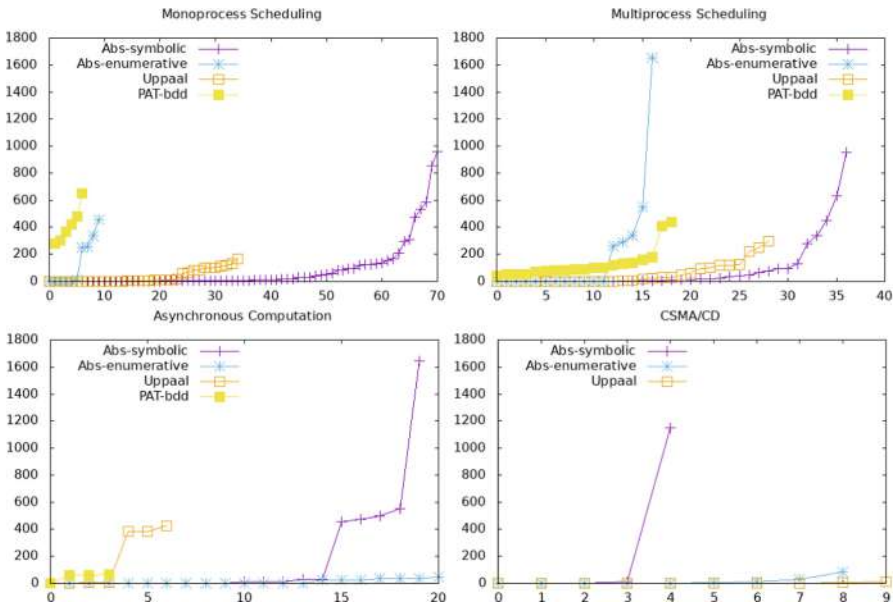


Fig. 3. Comparison of our enumerative and symbolic algorithms (referred to as Abs-enumerative and Abs-symbolic) with Uppaal and PAT. Each figure is a cactus plot for the set of benchmarks: a point (X, Y) means X benchmarks were solved within time bound Y.

6 Conclusion and Future Work

There are several ways to improve the algorithm. Since the choice of interpolants determines the abstraction function and the number of refinements, we assumed that taking the minimal interpolant should be preferable as it should keep the abstractions as coarse as possible. But it might be better to predict which interpolant is the most adapted for the rest of the computation in order to limit future refinements. The number of refinement also depends on the search order, and although it has already been studied in [23], it could be interesting to study it in this case. Generally speaking, it is worth noting that we currently cannot predict which (variant of) our algorithms is better suited for which model.

Several extensions of our algorithms could be developed, *e.g.* combining our algorithms with other methods based on finer abstractions as in [22], integrating predicate abstraction on discrete variables, or developing SAT-based versions of our algorithms.

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Fast Algorithms for Handling Diagonal Constraints in Timed Automata

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Abstract. A popular method for solving reachability in timed automata proceeds by enumerating reachable sets of valuations represented as zones. A naïve enumeration of zones does not terminate. Various termination mechanisms have been studied over the years. Coming up with efficient termination mechanisms has been remarkably more challenging when the automaton has diagonal constraints in guards.

In this paper, we propose a new termination mechanism for timed automata with diagonal constraints based on a new simulation relation between zones. Experiments with an implementation of this simulation show significant gains over existing methods.

Keywords: Timed automata · Diagonal constraints · Reachability · Zones · Simulations

1 Introduction

Timed automata have emerged as a popular model for systems with real-time constraints [2]. Timed automata are finite automata extended with real-valued variables called *clocks*. All clocks are assumed to start at 0, and increase at the same rate. Transitions of the automaton can make use of these clocks to disallow behaviours which violate timing constraints. This is achieved by making use of *guards* which are constraints of the form $x \leq 5$, $x - y \geq 3$, $y > 7$, etc. where x, y are clocks. A transition guarded by $x \leq 5$ says that it can be fired only when the value of clock x is ≤ 5. Another important feature is the *reset* of clocks in transitions. Each transition can specify a subset of clocks whose values become 0 once the transition is fired. The combination of guards and resets allows to track timing distance between events. A basic question that forms the core of timed automata technology is *reachability*: given a timed automaton, does there

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exist an execution from its initial state to a final state. This question is known to be decidable [2]. Various algorithms for this problem have been studied over the years and have been implemented in tools [6,21,26,28,31,32].

Since the clocks are real valued variables, the space of configurations of a timed automaton (consisting of a state and a valuation of the clocks) is infinite and an explicit enumeration is not possible. The earliest solution to reachability was to partition this space into a finite number of *regions* and build a region graph that provides a finite abstraction of the behaviour of the timed automaton [2]. However, this solution was not practical. Subsequent works introduced the use of *zones* [14]. Zones are special sets of clock valuations with efficient data structures and manipulation algorithms [6]. Within zone based algorithms, there is a division: forward analysis versus backward analysis. The current industry strength tool UPPAAL [28] implements a forward analysis approach, as this works better in the presence of other discrete data structures used in UPPAAL models [9]. We focus on this forward analysis approach using zones in this paper.

The forward analysis of a timed automaton essentially enumerates sets of reachable configurations stored as zones. Some extra care needs to be taken for this enumeration to terminate. Traditional development of timed automata made use of *extrapolation* operators over zones to ensure termination. These are functions which map a zone to a bigger zone. Importantly, the range of these functions is finite. The goal was to come up with extrapolation operators which are sound: adding these extra valuations should not lead to new behaviours. This is where the role of *simulations* between configurations was studied and extrapolation operators based on such simulations were devised [14]. A certain extrapolation operation, which is now known as Extra_M [5] was proposed and reachability using Extra_M was implemented in tools [14].

A seminal paper by Bouyer [9] revealed that Extra_M is not correct in the presence of *diagonal constraints* in guards. These are constraints of the form $x - y \triangleleft c$ where $\triangleleft$ is either $<$ or $\leq$, and c is an integer. Moreover, it was proved that no such extrapolation operation would be correct when there are diagonal constraints present. It was shown that for automata without diagonal constraints (henceforth referred to as diagonal-free automata), the extrapolation works. After this result, developments in timed automata reachability focussed on the class of diagonal-free automata [4,5,23,24], and diagonal constraints were mostly sidelined. All these developments have led to quite efficient algorithms for diagonal-free timed automata.

Diagonal constraints are a useful modeling feature and occur naturally in certain problems, especially scheduling [3,17,20,27] and logic-automata translations [16,25], also in [29]. It is however known that they do not add any expressive power: every timed automaton can be converted into a diagonal-free timed automaton [7]. This conversion suffers from an exponential blowup, which was later shown to be unavoidable: diagonal constraints could potentially give exponentially more succinct models [10]. Therefore, a good forward analysis algorithm that works directly on a timed automaton with diagonal constraints would be handy. This is the subject of this paper.

Related Work. The first attempt at such an algorithm was to split the (extrapolated) zones with respect to the diagonal constraints present in the automaton [6]. This gave a correct procedure, but since zones are split, an enumeration starts from each small zone leading to an exponential blow-up in the number of visited zones. A second attempt was to do a more refined conversion into a diagonal free automaton by detecting "relevant" diagonals [13,30] in an iterative manner. In order to do this, special data structures storing sets of sets of diagonal constraints were utilized. In [18] we extended the works [5] and [23] on diagonal-free automata to the case of diagonal constraints. All the approaches suffer from either a space or time bottleneck and are incomparable to the efficiency and scalability of tools for diagonal-free automata.

Our Contributions. The goal of this paper is to come up with fast algorithms for handling diagonal constraints. Since the extrapolation based approach is a dead end, we work with simulation between zones directly, as in [23] and [18]. We propose a new simulation relation between zones that is correct in the presence of diagonal constraints (Sect. 3). We give an algorithm to test this simulation between zones (Sect. 4). We have incorporated this simulation test in (an older version of) the tool TChecker [21] checking reachability for timed automata, and compared our results with the state-of-the-art tool UPPAAL. Experiments show an encouraging gain, both in the number of zones enumerated and in the time taken by the algorithm, sometimes upto four orders of magnitude (Sect. 6). The main advantage of our approach is that it does not split zones, and furthermore it leverages the optimizations studied for diagonal-free automata.

From a technical point of view, our presentation does not make use of regions and instead works with valuations, zones and simulation relations. We think that this presentation provides a clearer perspective - as a justification of this claim, we extend our simulation to timed automata with general updates of the form $x := c$ and $x := y + d$ in transitions (where x, y are clocks and c, d are constants) in a rather natural manner (Sect. 5). In general, reachability for timed automata with updates is undecidable [12]. Some decidable cases have been proposed for which the algorithms are based on regions. For decidable subclasses containing diagonal constraints, no zone based approach has been studied. Our proposed method includes these classes, and also benefits from zones and standard optimizations studied for diagonal-free automata.

Missing proofs can be found in the full version of this paper [19].

2 Preliminaries

Let $\mathbb{N}$ be the set of natural numbers, $\mathbb{R}_{\geq 0}$ the set of non-negative reals and $\mathbb{Z}$ the set of integers. Let X be a finite set of variables ranging over $\mathbb{R}_{\geq 0}$, called *clocks*. Let $\Phi(X)$ denote the set of constraints φ formed using the following grammar: $\varphi := x \lhd c \mid c \lhd x \mid x - y \lhd d \mid \varphi \wedge \varphi$, where $x, y \in X$, $c \in \mathbb{N}$, $d \in \mathbb{Z}$ and $\lhd \in \{<, \leq\}$. Constraints of the form $x \lhd c$ and $c \lhd x$ are called *non-diagonal constraints* and those of the form $x - y \lhd c$ are called *diagonal constraints*. We have adopted a convention that in non-diagonal constraints $x \lhd c$ and $c \lhd x$, the

constant c is restricted to $\mathbb{N}$. A *clock valuation* v is a function which maps every clock $x \in X$ to a real number $v(x) \in \mathbb{R}_{\geq 0}$. A valuation is said to satisfy a guard g, written as $v \models g$ if replacing every x in g with $v(x)$ makes the constraint g true. For $\delta \in \mathbb{R}_{\geq 0}$ we write $v + \delta$ for the valuation which maps every x to $v(x) + \delta$. Given a subset of clocks $R \subseteq X$, we write $[R]v$ for the valuation which maps each $x \in R$ to 0 and each $x \notin R$ to $v(x)$.

A *timed automaton* $\mathcal{A}$ is a tuple (Q, X, q_0, T, F) where Q is a finite set of states, X is a finite set of clocks, $q_0 \in Q$ is the initial state, $F \subseteq Q$ is a set of accepting states and $T \in Q \times \Phi(X) \times 2^X \times Q$ is a set of transitions. Each transition $t \in T$ is of the form (q, g, R, q') where q and q' are respectively the source and target states, g is a constraint called the *guard*, and R is a set of clocks which are *reset* in t. We call a timed automaton *diagonal-free* if guards in transitions do not use diagonal constraints.

A *configuration* of $\mathcal{A}$ is a pair (q, v) where $q \in Q$ and v is a valuation. The semantics of a timed automaton is given by a transition system $\mathcal{S}_\mathcal{A}$ whose states are the configurations of $\mathcal{A}$. Transitions in $\mathcal{S}_\mathcal{A}$ are of two kinds: *delay* transitions are given by $(q, v) \xrightarrow{\delta} (q, v + \delta)$ for all $\delta \geq 0$, and *action* transitions are given by $(q, v) \xrightarrow{t} (q', v')$ for each $t := (q, g, R, q')$, if $v \models g$ and $v' = [R]v$. We write $\xrightarrow{\delta,t}$ for a sequence of delay δ followed by action t. A run of $\mathcal{A}$ is an alternating sequence of delay-action transitions starting from the initial state q_0 and the initial valuation $\mathbf{0}$ which maps every clock to 0: $(q_0, \mathbf{0}) \xrightarrow{\delta_0,t_0} (q_1, v_1) \xrightarrow{\delta_1,t_1} \cdots (q_n, v_n)$. A run of the above form is said to be accepting if the last state $q_n \in F$. The *reachability problem* for timed automata is the following: given an automaton $\mathcal{A}$, decide if there exists an accepting run. This problem is known to be PSPACE-complete [2]. Since the semantics $\mathcal{S}_\mathcal{A}$ is infinite, solutions to the reachability problem work with a finite abstraction of $\mathcal{S}_\mathcal{A}$ that is sound and complete. Before we explain one of the popular solutions to reachability, we state a result which allows to convert every timed automaton into a diagonal-free timed automaton.

Theorem 1. *[7] For every timed automaton $\mathcal{A}$, there exists a diagonal-free timed automaton $\mathcal{A}_{df}$ s.t. there is a bijection between runs of $\mathcal{A}$ and $\mathcal{A}_{df}$. The number of states in $\mathcal{A}_{df}$ is $2^d \cdot n$ where d is the number of diagonal constraints and n is the number of states of $\mathcal{A}$.*

The above theorem allows to solve the reachability of a timed automaton $\mathcal{A}$ by first converting it into the diagonal free automaton $\mathcal{A}_{df}$ and then checking reachability on $\mathcal{A}_{df}$. However, this conversion comes with a systematic exponential blowup (in terms of the number of diagonal constraints present in $\mathcal{A}$). It was shown in [10] that such a blowup is unavoidable in general. We will now recall the general algorithm for analyzing timed automata, and then move into specific details which depend on whether the automaton has diagonal constraints or not.

Zones and Simulations. Fix a timed automaton $\mathcal{A}$ with clock set X for the rest of the discussion in this section. As the space of valuations of $\mathcal{A}$ is infinite, algorithms work with sets of valuations called *zones*. A zone is set of clock valuations given by a conjunction of constraints of the form $x - y \lhd c$, $x \lhd c$ and

$c \triangleleft x$ where $c \in \mathbb{Z}$ and $\triangleleft \in \{<, \leq\}$, for example the solutions of $x - y < 5 \wedge y \leq 10$ is a zone. The transition relation over configurations (q, v) is extended to (q, Z) where Z is a zone. We define the following operations on zones given a guard g and a set of clocks R: time elapse $\overrightarrow{Z} = \{v + \delta \mid v \in Z, \delta \geq 0\}$; guard intersection $Z \wedge g := \{v \mid v \in Z \text{ and } v \models g\}$ and reset $[R]Z := \{[R]v \mid v \in Z\}$. It can be shown that all these operations result in zones. Zones can be efficiently represented and manipulated using Difference Bound Matrices (DBMs) [15].

The *zone graph* $ZG(\mathcal{A})$ of timed automaton $\mathcal{A}$ is a transition system whose nodes are of the form (q, Z) where q is a state of $\mathcal{A}$ and Z is a zone. For each transition $t := (q, g, R, q')$ of $\mathcal{A}$, and each zone (q, Z) there is a transition $(q, Z) \Rightarrow^t (q', Z')$ where $Z' = \overrightarrow{[R](Z \wedge g)}$. The initial node is (q_0, Z_0) where q_0 is the initial state of $\mathcal{A}$ and $Z_0 = \{\mathbf{0} + \delta \mid \delta \geq 0\}$ is the zone obtained by elapsing an arbitrary delay from the initial valuation. A path in the zone graph is a sequence $(q_0, Z_0) \Rightarrow^{t_0} (q_1, Z_1) \Rightarrow^{t_1} \cdots \Rightarrow^{t_{n-1}} (q_n, Z_n)$ starting from the initial node. The path is said to be accepting if q_n is an accepting state. The zone graph is known to be sound and complete for reachability.

Theorem 2. *[14] $\mathcal{A}$ has an accepting run iff $ZG(\mathcal{A})$ has an accepting path.*

This does not yet give an algorithm as the zone graph $ZG(\mathcal{A})$ is still not finite. Moreover, there are examples of automata for which the reachable part of $ZG(\mathcal{A})$ is also infinite: starting from the initial node, applying the successor computation leads to infinitely many zones. Two different approaches have been studied to get finiteness, both of them based on the usage of *simulation relations*.

A (time-abstract) simulation relation ($\preccurlyeq$) between configurations of $\mathcal{A}$ is a reflexive and transitive relation such that $(q, v) \preccurlyeq (q', v')$ implies $q = q'$ and (1) for every $\delta \geq 0$, there exists $\delta' \geq 0$ such that $(q, v + \delta) \preccurlyeq (q, v' + \delta')$ and (2) for every transition t of $\mathcal{A}$, if $(q, v) \xrightarrow{t} (q_1, v_1)$ then $(q, v') \xrightarrow{t} (q_1, v_1')$ such that $(q_1, v_1) \preccurlyeq (q_1, v_1')$.

We say $v \preccurlyeq v'$, read as v is simulated by v' if $(q, v) \preccurlyeq (q, v')$ for all states q. The simulation relation can be extended to zones: $Z \preccurlyeq Z'$ if for every $v \in Z$ there exists $v' \in Z'$ such that $v \preccurlyeq v'$. We write $\downarrow Z$ for $\{v \mid \exists v' \in Z \text{ s.t. } v \preccurlyeq v'\}$. The simulation relation $\preccurlyeq$ is said to be finite if the function mapping zones Z to the down sets $\downarrow Z$ has finite range. We now recall a specific simulation relation $\preccurlyeq_{LU}$ [5,23]. Current algorithms and tools for diagonal-free automata are based on this simulation. The conditions required for $v \preccurlyeq_{LU} v'$ ensure that when all lower bound constraints $c \triangleleft x$ satisfy $c \leq L(x)$ and all upper bound constraints $x \triangleleft c$ satisfy $c \leq U(x)$, whenever v satisfies a constraint, v' will also satisfy it.

Definition 1 (LU-bounds and the relation $\preccurlyeq_{LU}$ [5,23]). *An LU-bounds function is a pair of functions $L : X \mapsto \mathbb{N} \cup \{-\infty\}$ and $U : X \mapsto \mathbb{N} \cup \{-\infty\}$ that map each clock to either a non-negative constant or $-\infty$. Given an LU-bounds function, we define $v \preccurlyeq_{LU} v'$ for valuations v, v' if for every clock $x \in X$:*

$$v'(x) < v(x) \text{ implies } L(x) < v'(x) \quad \text{and} \quad v(x) < v'(x) \text{ implies } U(x) < v(x).$$

Reachability in Diagonal-Free Timed Automata. A natural method to get finiteness of the zone graph is to prune the zone graph computation through simulations $Z \preccurlyeq Z'$: do not explore a node (q, Z) if there is an already visited node (q, Z') such that $Z \preccurlyeq Z'$. Since these simulation tests need to be done often during the zone graph computation, an efficient algorithm for performing this test is crucial. Note that $Z \preccurlyeq Z'$ iff $Z \subseteq \downarrow Z'$. However, it is known that the set $\downarrow Z'$ is not necessarily a zone (this was proved for $\downarrow_{LU} Z'$ in [5]), and hence no simple zone inclusions are applicable. The first algorithms for timed automata followed a different approach, which we call the *extrapolation* approach. In this approach, whenever a new zone Z is discovered by the algorithm, a new zone $\mathsf{Extra}(Z)(\supseteq Z)$ gets computed and stored in the place of Z.

Reachability Algorithm Using Zone Extrapolation. The input to the algorithm is a timed automaton $\mathcal{A}$. The algorithm maintains two lists, Passed and Waiting. Initially, the node $(q_0, \mathsf{Extra}(Z_0))$ is added to the Waiting list (recall that (q_0, Z_0) is the initial node of the zone graph $ZG(\mathcal{A})$). Wlog. we assume that q_0 is not accepting. The algorithm repeatedly performs the following steps:

Step 1. If Waiting is empty, then return "$\mathcal{A}$ has no accepting run"; else pick (and remove) a node (q, Z) from Waiting. Add (q, Z) to Passed.

Step 2. For each transition $t := (q, g, R, q_1)$, compute the successor $(q, Z) \Rightarrow^t (q_1, Z_1)$: if $Z_1 \neq \emptyset$ perform the following operations - if q_1 is accepting, return "$\mathcal{A}$ has an accepting run"; else compute $\hat{Z}_1 := \mathsf{Extra}(Z_1)$ and check if there exists a node (q_1, Z_1') in Passed or Waiting such that $\hat{Z}_1 \subseteq Z_1'$: if yes, ignore the node $(q_1, \hat{Z}_1)$, otherwise add $(q_1, \hat{Z}_1)$ to Waiting.

Several extrapolation operators (Extra_M, Extra_{LU}, Extra^+_{LU}) were introduced in [5]. The function Extra^+_{LU} has nice properties - (1) $\mathsf{Extra}^+_{LU}(Z) \subseteq \downarrow_{LU} Z$ and (2) $\mathsf{Extra}^+_{LU}(Z)$ is a zone for all Z. These properties give an algorithm that performs only efficient zone operations: successor computations and zone inclusions.

Reachability Algorithm Using Simulations. The initial node (q_0, Z_0) is added to the Waiting list. Wlog. we assume that q_0 is not accepting. The algorithm repeatedly performs the following steps:

Step 1. If Waiting is empty, then return "$\mathcal{A}$ has no accepting run"; else pick (and remove) a node (q, Z) from Waiting. Add (q, Z) to Passed.

Step 2. For each transition $t := (q, g, R, q_1)$, compute the successor $(q, Z) \Rightarrow^t (q_1, Z_1)$: if $Z_1 \neq \emptyset$ perform the following operations - if q_1 is accepting, return "$\mathcal{A}$ has an accepting run"; else check if there exists a node (q_1, Z_1') in Passed or Waiting such that $Z_1 \preccurlyeq Z_1'$: if yes, ignore the node (q_1, Z_1), otherwise add (q_1, Z_1) to Waiting.

An $\mathcal{O}(|X|^2)$ algorithm for $Z \preccurlyeq_{LU} Z'$ was proposed in [23]. The efficiency of this simulation check makes it well suited for use in practice. Moreover, as $\mathsf{Extra}^+_{LU}(Z) \subseteq \downarrow_{LU} Z$, we expect to get more simulations (and hence quicker termination) through $\preccurlyeq_{LU}$.

Reachability in the Presence of Diagonal Constraints. The $\preccurlyeq_{LU}$ relation is no longer a simulation when diagonal constraints are present. Moreover, it was shown in [9] that no extrapolation operator (along the lines of Extra^{+}_{LU}) can work in the presence of diagonal constraints. The first option to deal with diagonals is to use Theorem 1 to get a diagonal free automaton and then apply the methods discussed previously. One problem with this is the systematic exponential blowup introduced in the number of states of the resulting automaton. Another problem is to get diagnostic information: counterexamples need to be translated back to the original automaton [6]. Various methods have been studied to circumvent the diagonal free conversion and instead work on the automaton with diagonal constraints directly. We recall the approach used in the state-of-the-art tool UPPAAL below.

Zone Splitting [6]. The paper introducing timed automata gave a notion of equivalence between valuations $v \simeq_M v'$ parameterized by a function M mapping each clock x to the maximum constant M among the guards of the automaton that involve x. This equivalence is a finite simulation for diagonal-free automata. Equivalence classes of $\simeq_M$ are called regions. This was extended to the diagonal case by [6] as: $v \simeq^d_M v'$ if $v \simeq_M v'$ and for all diagonal constraints g present in the automaton, if $v \models g$ then $v' \models g$. The $\simeq^d_M$ relation splits the regions further, such that each region is either entirely included inside g, or entirely outside g for each g. The next step is to use this notion of equivalence in zones. The paper [6] follows the extrapolation approach: to each zone Z, an extrapolation operation $\mathsf{Extra}_M(Z)$ is applied; this adds some valuations which are $\simeq_M$ equivalent to valuations in Z; then it is further split into multiple zones, so that each small zone is either inside g or outside g for each diagonal constraint g. If d is the number of diagonal constraints present in the automaton, this splitting process can give rise to 2^d zones for each zone Z. From each small zone, the zone graph computation is started. Essentially, the exponential blow-up at the state level which appeared in the diagonal-free conversion now appears in the zone level.

In this paper, we propose a new simulation to handle diagonal constraints. This has two advantages - using this avoids the blow-up in the number of nodes arising due to zone splitting, and the simulation test between zones has an efficient implementation and is significantly quicker than the simulation of [18].

3 A New Simulation Relation

We start with a definition of a relation between timed automata configurations, which in some sense "declares" upfront what we need out of a simulation relation that can be used in a reachability algorithm. As we proceed, we will make its description more concrete and give an effective simulation algorithm between zones, that can be implemented. Fix a clock set X. This generates constraints $\Phi(X)$.

Definition 2 (the relation $\sqsubseteq_{\mathcal{G}}$). *Let $\mathcal{G}$ be a (finite or infinite) set of constraints. We say $v \sqsubseteq_{\mathcal{G}} v'$ if for all $\varphi \in \mathcal{G}$ and all $\delta \geq 0$, $v + \delta \models \varphi$ implies $v' + \delta \models \varphi$.*

Our goal is to utilize the above relation in a simulation (as defined in p. xx) for a timed automaton. Directly from the definition, we get the following lemma which shows that the $\sqsubseteq_{\mathcal{G}}$ relation is preserved under time elapse.

Lemma 1. *If $v \sqsubseteq_{\mathcal{G}} v'$, then $v + \delta \sqsubseteq_{\mathcal{G}} v' + \delta$ for all $\delta \geq 0$.*

The other kind of transformation over valuations is resets. Given sets of guards $\mathcal{G}_1$, $\mathcal{G}$ and a set of clocks R, we want to find conditions on $\mathcal{G}_1$ and $\mathcal{G}$ so that if $v \sqsubseteq_{\mathcal{G}_1} v'$ then $[R]v \sqsubseteq_{\mathcal{G}} [R]v'$. To do this, we need to answer this question: what guarantees should we ensure for v, v' (via $\mathcal{G}_1$) so that $[R]v \sqsubseteq_{\mathcal{G}} [R]v'$. This motivates the next definition.

Definition 3 (weakest pre-condition of $\sqsubseteq_{\mathcal{G}}$ over resets). *For a constraint φ and a set of clocks R, we define a set of constraints $\mathrm{wp}(\sqsubseteq_{\varphi}, R)$ as follows: when φ is of the form $x \lhd c$ or $c \lhd x$, then $\mathrm{wp}(\sqsubseteq_{\varphi}, R)$ is empty if $x \in R$ and is $\{\varphi\}$ otherwise; when φ is a diagonal constraint $x - y \lhd c$, then $\mathrm{wp}(\sqsubseteq_{\varphi}, R)$ is:*

- $\{x - y \lhd c\}$ *if* $\{x, y\} \cap R = \emptyset$
- $\{x \lhd c\}$ *if* $y \in R$, $x \notin R$ *and* $c \geq 0$
- $\{-c \lhd y\}$ *if* $x \in R$, $y \notin R$ *and* $-c \geq 0$
- *empty, otherwise.*

For a set of guards $\mathcal{G}$, we define $\mathrm{wp}(\sqsubseteq_{\mathcal{G}}, R) := \bigcup_{\varphi \in \mathcal{G}} \mathrm{wp}(\sqsubseteq_{\varphi}, R)$.

Note that the relation $\sqsubseteq_{\mathcal{G}}$ is parameterized by a set of constraints. Additionally, we desire this set to be finite, so that the relation can be used in an algorithm. We need to first link an automaton $\mathcal{A}$ with such a set of constraints. One way to do it is to take the set of all guards present in the automaton and to close it under weakest pre-conditions with respect to all possible subsets of clocks. A better approach is to consider a set of constraints for each state, as in [4] where the parameters for extrapolation (the maximum constants appearing in guards) are calculated at each state.

Definition 4 (State based guards). *Let $\mathcal{A} = (Q, X, q_0, T, F)$ be a timed automaton. We associate a set of guards $\mathcal{G}(q)$ for each state $q \in Q$, which is the least set of guards (for the coordinate-wise subset inclusion order) such that for every transition (q, g, R, q_1): the guard g and the set $\mathrm{wp}(\sqsubseteq_{\mathcal{G}(q_1)}, R)$ are present in $\mathcal{G}(q)$. More precisely, $\{\mathcal{G}(q)\}_{q \in Q}$ is the least solution to the following set of equations written for each $q \in Q$:*

$$\mathcal{G}(q) = \bigcup_{(q,g,R,q_1) \in T} \{g\} \cup \mathrm{wp}(\sqsubseteq_{\mathcal{G}(q_1)}, R)$$

All constraints present in the set $\mathrm{wp}(\sqsubseteq_{\mathcal{G}(q_1)}, R)$ contain constants which are already present in $\sqsubseteq_{\mathcal{G}(q_1)}$. The least solution to the above set of equations can therefore be obtained by a fixed point computation which starts with $\mathcal{G}(q)$ set to $\bigcup_{(q,g,R,q_1) \in T} \{g\}$ and then repeatedly updates the weakest-preconditions. Since no new constants are generated in this process, the fixed point computation terminates. We now have the ingredients to define a simulation relation over configurations of a timed automaton with diagonal constraints.

Definition 5 ($\mathcal{A}$-simulation). *Let $\mathcal{A} = (Q, X, q_0, T, F)$ be a timed automaton and let the set of guards $\mathcal{G}(q)$ of Definition 4 be associated to every state $q \in Q$. We define a relation $\preccurlyeq_{\mathcal{A}}$ between configurations of $\mathcal{A}$ as $(q, v) \preccurlyeq_{\mathcal{A}} (q, v')$ if $v \sqsubseteq_{\mathcal{G}(q)} v'$.*

Lemma 2. *The relation $\preccurlyeq_{\mathcal{A}}$ is a simulation on the configurations of timed automaton $\mathcal{A}$.*

As pointed before, Definition 2 gives a declarative description of the simulation and it is unclear how to work with it algorithmically, even when the set of constraints $\mathcal{G}$ is finite. The main issue is with the $\forall\delta$ quantification, which is not finite. We will first provide a characterization that brings out the fact that this $\forall\delta$ quantification is irrelevant for diagonal constraints (essentially because value of $v(x) - v(y)$ does not change with time elapse). Given a set of constraints $\mathcal{G}$, let $\mathcal{G}^- \subseteq \mathcal{G}$ be the set of non-diagonal constraints in $\mathcal{G}$.

Proposition 1. *$v \sqsubseteq_{\mathcal{G}} v'$ iff $v \sqsubseteq_{\mathcal{G}^-} v'$ and for all diagonal constraints $\varphi \in \mathcal{G}$, if $v \models \varphi$ then $v' \models \varphi$.*

It now amounts to solving the $\forall\delta$ problem for non-diagonals. It turns out that the $\preccurlyeq_{LU}$ simulation achieves this, almost. We will see this in more detail in the next section.

4 Algorithm for $Z \sqsubseteq_{\mathcal{G}} Z'$

Fix a finite set of guards $\mathcal{G}$. Restating the definition of $\sqsubseteq_{\mathcal{G}}$ extended to zones: $Z \sqsubseteq_{\mathcal{G}} Z'$ if for all $v \in Z$ there exists a $v' \in Z'$ such that $v \sqsubseteq_{\mathcal{G}} v'$. In this section, we will view the characterization of $\sqsubseteq_{\mathcal{G}}$ as in Proposition 1 and give an algorithm to check $Z \sqsubseteq_{\mathcal{G}} Z'$ that uses as an oracle a test $Z \sqsubseteq_{\mathcal{G}^-} Z'$. We discuss the computation of $Z \sqsubseteq_{\mathcal{G}^-} Z'$ later in this section. We start with an observation following from Proposition 1.

Lemma 3. *Let $\varphi := x - y \lhd c$ be a diagonal constraint in $\mathcal{G}$. Then $Z \sqsubseteq_{\mathcal{G}} Z'$ if and only if $Z \cap \varphi \sqsubseteq_{\mathcal{G}'} Z' \cap \varphi$ and $Z \cap \neg\varphi \sqsubseteq_{\mathcal{G}'} Z'$ where $\mathcal{G}' = \mathcal{G} \setminus \{\varphi\}$.*

If $\mathcal{G}$ has no diagonal constraints, $Z \sqsubseteq_{\mathcal{G}} Z'$ if and only if $Z \sqsubseteq_{\mathcal{G}^-} Z'$.

This leads to the following algorithm consisting of two mutually recursive procedures. This algorithm is essentially an implementation of the above lemma, with two optimizations:

- we start with the non-diagonal check in Line 6 of Algorithm 1 - if this is already violated, then the algorithm returns false;
- suppose $Z \sqsubseteq_{\mathcal{G}^-} Z'$, the next task is to perform the checks in the first statement of Lemma 3 - this is done by Algorithm 2; note however that when Algorithm 2 is called, we already have $Z \sqsubseteq_{\mathcal{G}^-} Z'$, hence $Z \cap \neg\varphi \sqsubseteq_{\mathcal{G}^-} Z'$. Therefore we use an optimization in Line 7 by calling Algorithm 2 directly (as the check in Line 6 of Algorithm 1 will be redundant).

```
1 check Z ⊑_G Z':
2     if Z = ∅ :
3         return true
4     if Z' = ∅ :
5         return false
6     if Z ⋢_{G⁻} Z' :
7         return false
8     return Z ⊑*_G Z'
```

Algorithm 1

```
1 check Z ⊑*_G Z':
2     if G does not contain any
      diagonal constraints :
3         return true
4     pick a diagonal constraint
      φ = x − y ◁ c from G
5     G' ⟵ G \ {φ}
6     if Z ∩ ¬φ ≠ ∅ :
7         if Z ∩ ¬φ ⋢*_{G'} Z' :
8             return false
9     return Z ∩ φ ⊑_{G'} Z' ∩ φ
```

Algorithm 2

Computing $Z \sqsubseteq_{\mathcal{G}^-} Z'$. We will use $\preccurlyeq_{LU}$ to approximate $\sqsubseteq_{\mathcal{G}^-}$: in our implementation of the above algorithms, we replace $Z \sqsubseteq_{\mathcal{G}^-} Z'$ with $Z \preccurlyeq_{LU} Z'$. This works because for an appropriate choice of LU (explained below), we have $Z \preccurlyeq_{LU(\mathcal{G})} Z' \Rightarrow Z \sqsubseteq_{\mathcal{G}^-} Z'$. The converse is not true as the LU bounds functions cannot distinguish between guards with $<$ and $\leq$ comparisons. Therefore, the $\preccurlyeq_{LU}$ simulation does not characterize $v \sqsubseteq_{\mathcal{G}^-} v'$ completely. Although we are aware of the (rather technical) modifications to $\preccurlyeq_{LU}$ simulation that are needed for this characterization, we choose to use the existing $\preccurlyeq_{LU}$ directly as it is safe to do so and it has already been implemented in tools. This gives us a finer simulation than $v \sqsubseteq_{\mathcal{G}^-} v'$.

Definition 6 (LU-bounds from $\mathcal{G}$). *Let $\mathcal{G}$ be a finite set of constraints. We define $LU(\mathcal{G})$ to denote the pair of functions $L_{\mathcal{G}}$ and $U_{\mathcal{G}}$ defined as follows:*

$$L_{\mathcal{G}}(x) = \begin{cases} -\infty & \text{if there is no guard of the form } c \lhd x \text{ in } \mathcal{G} \\ \max\{c \mid c \lhd x \in \mathcal{G}\} & \text{otherwise} \end{cases}$$

$$U_{\mathcal{G}}(x) = \begin{cases} -\infty & \text{if there is no guard of the form } x \lhd c \text{ in } \mathcal{G} \\ \max\{c \mid x \lhd c \in \mathcal{G}\} & \text{otherwise} \end{cases}$$

Lemma 4. *For every set of constraints $\mathcal{G}$, $v \preccurlyeq_{LU(\mathcal{G})} v'$ implies $v \sqsubseteq_{\mathcal{G}^-} v'$.*

The above observations call for the next definition and subsequent lemmas.

Definition 7 (approximating $\sqsubseteq_{\mathcal{G}}$). *Let $\mathcal{G}$ be a finite set of constraints. We define a relation $\sqsubseteq^{LU}_{\mathcal{G}}$ as follows: $v \sqsubseteq^{LU}_{\mathcal{G}} v'$ if $v \preccurlyeq_{LU(\mathcal{G})} v'$ and for all diagonal constraints $\varphi \in \mathcal{G}$, if $v \models \varphi$ then $v' \models \varphi$. Similarly, define $\preccurlyeq^{LU}_{\mathcal{A}}$ as $(q, v) \preccurlyeq^{LU}_{\mathcal{A}} (q, v')$ if $v \sqsubseteq^{LU}_{\mathcal{G}(q)} v'$.*

Lemma 5. *The relation $\preccurlyeq^{LU}_{\mathcal{A}}$ is a finite simulation on the configurations of $\mathcal{A}$.*

The above lemma and the fact that $Z \preccurlyeq_{LU(\mathcal{G})} Z'$ can be checked in $\mathcal{O}(|X|^2)$ [23,33], imply the following theorem.

Theorem 3. *When using $Z \preccurlyeq_{LU(\mathcal{G})} Z'$ in the place of $Z \sqsubseteq_{\mathcal{G}^-} Z'$, the algorithm is correct and it terminates in $\mathcal{O}(2^d \cdot |X|^2)$ where d is the number of diagonal guards in $\mathcal{G}$.*

From a complexity viewpoint, this algorithm is not efficient since it makes an exponential number of calls in the number of diagonal constraints (in fact this may not be avoidable due to Lemma 6, which follows from the NP-hardness result in [18]). Although the above algorithm does involve many calls, the internal operations involved in each call are simple zone manipulations. Moreover, the preliminary checks (for instance line 6 of Algorithm 1) cut short the number of calls. This is visible in our experiments which are very good, especially with respect to running time, as compared to other methods. A similar hardness was shown for a different simulation in [18], but the implementation there indeed witnessed the hardness, as the time taken by that algorithm was unsatisfactory.

Lemma 6. *Deciding $Z \not\sqsubseteq^{LU}_{\mathcal{G}} Z'$ is NP-complete.*

5 Simulations for Updatable Timed Automata

In the timed automata considered so far, clocks are allowed to be reset to 0 along transitions. We consider in this section more sophisticated transformations to clocks in transitions. These are called *updates*. An update $up : \mathbb{R}^{|X|}_{\geq 0} \mapsto \mathbb{R}^{|X|}$ is a function mapping non-negative $|X|$-dimensional reals (valuations) v to general $|X|$-dimensional reals (which may apriori not be valuations as the coordinates may be negative). The syntax of the update function up is given by a set of atomic updates up_x to each $x \in X$, which are of the form $x := c$ or $x := y + d$ where $c \in \mathbb{N}$, $d \in \mathbb{Z}$ and $y \in X$ (possibly equal to x). Note that we want d to be an integer, since we allow for decrementing clocks, and on the other hand $c \in \mathbb{N}$ since we have non-negative clocks. Given a valuation v and an update up, the valuation $up(v)$ is:

$$up(v)(x) := \begin{cases} c & \text{if } up_x \text{ is } x := c \\ v(y) + d & \text{if } up_x \text{ is } x := y + d \end{cases}$$

Note that in general, due to the presence of updates $x := y+d$, the update $up(v)$ may not yield a clock valuation. However, when it does give a valuation, it can be used as a transformation in timed automata transitions. We say $up(v) \geq 0$ if $up(v)(x) \geq 0$ for all clocks $x \in X$.

An *updateable timed automaton (UTA)* $\mathcal{A} = (Q, X, q_0, T, F)$ is an extension of a classic timed automaton with transitions of the form (q, g, up, q') where up is an update. Semantics extend in the natural way: delay transitions remain the same, and for action transitions $t := (q, g, up, q')$ we have $(q, v) \xrightarrow{t} (q', v')$ if $v \models g$, $up(v) \geq 0$, and $v' = up(v)$. We allow the transition only if the update results

in a valuation. The reachability problem for these automata is known to be undecidable in general [12]. Various subclasses with decidable reachability have been discussed in the same paper. Decidability proofs in [12] take the following flavour, for a given automaton $\mathcal{A}$: (1) divide the space of all valuations into a finite number of equivalence classes called *regions* (2) to build the parameters for the equivalence, derive a set of diophantine equations from the guards of $\mathcal{A}$; if they have a solution then construct the quotient graph of the equivalence (called region graph) parameterized by the obtained solution and check reachability on it; if the equations have no solution, output that reachability for $\mathcal{A}$ cannot be answered. Sufficient conditions on the nature of the updates that give a solution to the diophantine equations have been tabulated in [12]. When the automaton is diagonal-free, the "region-equivalence" can be used to build an extrapolation operation which in turn can be used in a reachability algorithm with zones. When the automaton contains diagonals, the region-equivalence is used to only build a region graph - no effective zone based approach has been studied.

We use a similar idea, but we have two fundamental differences: (1) we want to obtain reachability through the use of simulations on zones, and (2) we build equations over sets of guards as in Definition 4. The advantage of this approach is that this allows the use of coarser simulations over zones. Even for automata with diagonal constraints and updates, we get a zone based algorithm, instead of resorting to regions which are not efficient in practice.

The notion of simulations as in p. xx remains the same, now using the semantics of transitions with updates. We will re-use the simulation relation $\sqsubseteq_{\mathcal{G}}$. We need to extend Definition 3 to incorporate updates. We do this below. Here is a notation: for an update function up, we write $up(x)$ to be c if up_x is $x := c$, and $up(x)$ to be $y + c$ if up_x is $x := y + c$.

Definition 8 (weakest pre-condition of $\sqsubseteq_{\mathcal{G}}$ over updates).
Let up be an update.

For a constraint φ of the form $x \lhd c$ or $c \lhd x$, we define $\mathrm{wp}(\sqsubseteq_\varphi, up)$ *to be respectively* $\{up(x) \lhd c\}$ *or* $\{c \lhd up(x)\}$ *if these resulting constraints are of the form $z \lhd d$ or $d \lhd z$ with $z \in X$ and $d \geq 0$, otherwise* $\mathrm{wp}(\sqsubseteq_\varphi, up)$ *is empty.*

For a constraint $\varphi : x - y \lhd c$, we define $\mathrm{wp}(\sqsubseteq_\varphi, up)$ *to be* $\{up(x) - up(y) \lhd c\}$ *if this constraint is either a diagonal using different clocks, or it is of the form $z \lhd d$ or $d \lhd z$ with $d \geq 0$, otherwise* $\mathrm{wp}(\sqsubseteq_\varphi, up)$ *is empty.*

For a set of guards $\mathcal{G}$, we define $\mathrm{wp}(\sqsubseteq_{\mathcal{G}}, up) := \bigcup_{\varphi \in \mathcal{G}} \mathrm{wp}(\sqsubseteq_\varphi, up)$.

Some examples: $\mathrm{wp}(x \leq 5, x := x + 10)$ is empty, since $up(x)$ is $x + 10$, and the guard $x + 10 \leq 5$ is not satisfiable; $\mathrm{wp}(x \leq 5, x := x - 10)$ is $x \leq 15$, $\mathrm{wp}(x \leq 5, x := c)$ is empty, $\mathrm{wp}(x - y \leq 5, \langle x := z_1, y := z_2 + 10\rangle)$ will be $z_1 - (z_2 + 10) \leq 5$, giving the constraint $z_1 - z_2 \leq 15$, $\mathrm{wp}(x - y \leq 5, \langle x := z + c_1, y := z + c_2\rangle)$ is empty, $\mathrm{wp}(x - y \leq 5, \langle x := c_1, y := z + c_2\rangle)$ is $c = c_1 - 5 - c_2 \leq z$ if $c \geq 0$ and is empty otherwise.

Definition 9 (State based guards). *Let $\mathcal{A} = (Q, X, q_0, T, F)$ be a UTA. We associate a set of constraints $\mathcal{G}(q)$ for each state $q \in Q$, which is the least set of constraints (for the coordinate-wise subset inclusion order) such that for*

every transition (q, g, up, q_1)*: the guard* g *and the set* $\mathrm{wp}(\sqsubseteq_{\mathcal{G}(q_1)}, up)$ *are present in* $\mathcal{G}(q)$*, and in addition constraints that allow the update to happen are also present in* $\mathcal{G}$*. The last condition is given by the weakest precondition of the set of constraints* $\{x \geq 0 \mid x \in X\}$*. Overall,* $\{\mathcal{G}(q)\}_{q\in Q}$ *is the least solution to the following set of equations, for each* $q \in Q$*:*

$$\mathcal{G}(q) = \bigcup_{(q,g,up,q_1)\in T} \left(\{g\} \cup \mathrm{wp}(\sqsubseteq_{\{x\geq 0 | x\in X\}}, up) \cup \mathrm{wp}(\sqsubseteq_{\mathcal{G}(q_1)}, up) \right)$$

The least solution $\{\mathcal{G}(q)\}_{q\in Q}$ *is said to be finite if each* $\mathcal{G}(q)$ *is a finite set of constraints.*

In contrast to the simple reset case, the above set of equations may not have a finite solution. Consider a self-looping transition: $(q, x \lhd c, x := x - 1, q)$. We require $x \lhd c \in \mathcal{G}(q)$. Now, $\mathrm{wp}(x \lhd c, x := x - 1)$ is $x \lhd c + 1$ which should be in $\mathcal{G}(q)$ according to the above equation. Continuing this process, we need to add $x \lhd d$ for every natural number $d \geq c$. Indeed this is consistent with the undecidability of reachability when subtraction updates are allowed. We deal with the subject of finite solutions to the above equations later in this section. On the other hand, when the above system does have a solution with finite $\mathcal{G}(q)$ at every q, we can use the $\mathcal{A}$ simulation of Definition 5 and its approximation $\preccurlyeq^{LU}_{\mathcal{A}}$ to get an algorithm.

Proposition 2. *Let* $\mathcal{A} = (Q, X, q_0, T, F)$ *be a UTA. Let* $\{\mathcal{G}(q)\}_{q\in Q}$ *be the least solution to the equations given in Definition 9. Then, the relation* $\preccurlyeq_{\mathcal{A}}$ *is a simulation on the configurations of* $\mathcal{A}$*.*

Lemma 7. *For a UTA* $\mathcal{A}$*, assume that the least solution* $\{\mathcal{G}(q)\}_{q\in Q}$ *to the state-based guards equations is finite. Then the relation* $\preccurlyeq^{LU}_{\mathcal{A}}$ *is a finite simulation on the configurations of* $\mathcal{A}$*.*

Finite Solution to the State-Based Guards Equations. The least solution to the equations of Definition 9 can be obtained by a standard Kleene iteration for fixed points computation. For each $i \geq 0$ and each state q, define:

$$\mathcal{G}^0(q) = \bigcup_{(q,g,up,q')\in T} \{g\} \cup \mathrm{wp}(\sqsubseteq_{\{x\geq 0 | x\in X\}}, up)$$

$$\mathcal{G}^{i+1}(q) = \bigcup_{(q,g,up,q')\in T} \mathcal{G}^i(q) \cup \mathrm{wp}(\sqsubseteq_{\mathcal{G}^i(q')}, up)$$

The iteration stabilizes when there exists a k satisfying $\mathcal{G}^{k+1}(q) = \mathcal{G}^k(q)$ for all q. At stabilization, the values $\mathcal{G}^k(q)$ satisfy the equations of Definition 9, and give the required $\mathcal{G}(q)$. However, as we mentioned earlier, this iteration might not stabilize at any k. We will now develop some observations that will help detect after finitely many steps if the iteration will stabilize or not.

Suppose we colour the set $\mathcal{G}^{i+1}(q)$ to *red* if either there exists a diagonal constraint $x - y \lhd c \in \mathcal{G}^{i+1}(q) \setminus \mathcal{G}^i(q)$ (a new diagonal is added) or there exists a

non-diagonal constraint $x \triangleleft c$ or $c \triangleleft x$ in $\mathcal{G}^{i+1}(q) \setminus \mathcal{G}^i(q)$ such that the constant c is strictly bigger than c' for respectively every non-diagonal $x \triangleleft c'$ or $c' \triangleleft x$ in $\mathcal{G}^i(q)$ (a non-diagonal with a bigger constant is added). If this condition is not applicable, we colour the set $\mathcal{G}^{i+1}(q)$ *green*. The next observations say that the iteration terminates iff we reach a stage where all sets are green. Intuitively, once we reach green, the only constraints that can be added are non-diagonals having smaller (non-negative) constants and hence the procedure terminates.

Lemma 8. *Let $i > 0$. If $\mathcal{G}^i(q)$ is green for all q, then $\mathcal{G}^{i+1}(q)$ is green for all q.*

Lemma 9. *Let $K = 1 + |Q| \cdot |X| \cdot (|X| + 1)$. If there is a state p such that $\mathcal{G}^K(p)$ is red, then there is no i such that $\mathcal{G}^i(q)$ is green for all q.*

As to why the bound $K = 1 + |Q| \cdot |X| \cdot (|X| + 1)$ in the lemma above: a red state at stage i arises due to the addition of a constraint φ_i at state p_i, which in turn depends on a state p_{i-1} marked red at stage $i-1$ due to constraint φ_{i-1}. If we iterate sufficiently long, we will hit a state p, a sequence of transitions from p to p and a constraint φ such that computing the weakest precondition over this loop will give a new constraint with the same set of clocks as φ but with a different constant. This part can be iterated infinitely often.

Proposition 3. *The least solution of the local constraint equations for a UTA is finite iff $\mathcal{G}^K(q)$ is green for all q and where $K = 1 + |Q| \cdot |X| \cdot (|X| + 1)$.*

Theorem 4. *Let $\mathcal{A}$ be a UTA. It is decidable whether the equations in Definition 9 have a finite solution. When these equations do have a finite solution, zone graph enumeration using $\preccurlyeq_{\mathcal{A}}^{LU}$ is a sound, complete and terminating procedure for the reachability problem.*

All decidable classes of [12] can be shown decidable with our approach, by showing stabilization of the $\mathcal{G}(q)$ computation.

Lemma 10. *Reachability is decidable in UTA where: guards are non-diagonals and updates are of the form $x := c$, $x := y$, $x := y + c$ where $c \geq 0$ or, guards include diagonal constraints and updates are of the form $x := c$, $x := y$.*

6 Experiments

We have implemented the reachability algorithm for timed automata with diagonal constraints (and only resets as updates) based on the simulation approach (p. xx) using the $\preccurlyeq_{\mathcal{A}}^{LU}$ simulation (Definition 7) for pruning zones. The algorithm for $Z \sqsubseteq_{\mathcal{G}}^{LU} Z'$ comes from Sect. 4. Experiments are reported in Table 1. We take model *Cex* from [8,30] and *Fischer* from [30]. We are not aware of any other "standard" benchmarks containing diagonal constraints. In addition to these two models, we introduce a new benchmark. This is an extension of the job-shop scheduling using (diagonal-free) timed automata [1]. Here the tasks within a job were logically independent. We add some timing dependency between them

Table 1. Experiments: the column $\#\mathcal{D}$ gives the number of diagonal constraints. Four methods have been reported in the table. First two methods, TChecker with our simulation relation $\sqsubseteq_{\mathcal{G}}^{LU}$ and UPPAAL engine for diagonals, have been run on $\mathcal{A}$, the automata containing diagonal constraints. Whereas, the third and fourth methods are running diagonal-free engines of UPPAAL and TChecker on $\mathcal{A}_{df}$, a diagonal-free equivalent of $\mathcal{A}$. Experiments were run on macOS X with 2.3 GHz Intel core i5 processor, and 8 GB RAM. Time is reported in seconds. We set a timeout of 15 min.

Model	$\#\mathcal{D}$	$\mathcal{A}$: contains diagonals				$\mathcal{A}_{df}$: diagonal-free *equivalent* of $\mathcal{A}$			
		TChecker + $\sqsubseteq_{\mathcal{G}}^{LU}$		UPPAAL		UPPAAL		TChecker	
		Time	Nodes count	Time	Nodes count	Time	Nodes count	Time	Nodes count
Cex 2	4	0.047	241	0.026	2180	0.005	1039	0.067	1039
Cex 3	6	7.399	7111	111.168	182394	1.028	60982	40.092	60982
Cex 4	8	857.662	185209	Timeout	-	734.543	3447119	Timeout	-
Fischer 4	4	0.032	452	307.836	357687	0.009	1815	0.100	1815
Fischer 5	5	0.257	1842	Timeout	-	0.116	12511	1.856	12511
Fischer 7	7	15.032	26812	Timeout	-	174.560	693603	Timeout	-
Job Shop 3	12	0.420	278	23.093	31711	0.003	845	0.312	845
Job Shop 5	20	285.421	10592	Timeout	-	4.633	179607	150.811	179607

which gets naturally modeled using diagonal constraints. Each model considered above is a product of a number of k timed automata. In the table we write the name of the model and the number k of automata involved in the product. We also report the number of diagonal constraints in each of them.

Experimental Results. We report the results of four methods of handling diagonal constraints, as mentioned in the caption of Table 1. Under each method, we report on the number of zones enumerated and the time taken. The first method gives a huge gain over the second one (upto four orders of magnitude in the number of nodes, and even better for time) and gives a less marked, but still significant, gain over the third and fourth methods. We provide a brief explanation of this phenomenon. The performance of the reachability algorithm is dependent on three factors:

- parameters of extrapolation or simulation: M-simulations which use the maximum constant appearing in the guards, versus the LU-simulations which make a distinction between lower bound guards $c \lhd x$ and upper bound guards $x \lhd c$ (refer to [5] for the exact definitions of extrapolations based on these parameters, and [23] for simulations based on these parameters); LU-simulations are superior to M-simulations.
- computation of the parameters: global parameters which associate a bound to each clock versus the more local state based parameters as in Definition 4 which associate a set of bounds functions to each state [4]; local bounds are superior to global bounds.
- when diagonal constraints are present, whether zones get split or not: each time a zone gets split, new enumerations start from each of the new nodes; clearly, a no-splitting-of-zones approach is superior to zone splitting.

Algorithm of column 1 uses the superior heuristic in all the three optimizations above. The no-splitting-of-zones was possible thanks to our simulation approach, which temporarily splits zones for checking $Z \sqsubseteq_G^{LU} Z'$, but never starts a new exploration from any of the split nodes. The algorithm of column 2, which is implemented in the current version UPPAAL 4.1 uses the inferior heuristic in all the three above. In particular, it is not clear how the extrapolation approach can avoid the zone splitting in an efficient manner. The superiority of our approach gets amplified (by multiplicative factors) when we consider bigger products with many more diagonals. In the third and fourth methods, we give a diagonal free equivalent of the original model (c.f. Theorem 1) and use the UPPAAL and TChecker engines respectively, for diagonal free timed automata. The UPPAAL diagonal free engine is highly optimized, and makes use of the superior heuristics in the first two optimizations mentioned above (the third heuristic is not applicable now as it is a diagonal free automaton). The third and fourth methods can be considered as a good approximation of the zone splitting approach to diagonal constraints using LU-abstractions and local guards.

The second and the third methods are the only possibilities of verifying timed models coming with diagonal constraints in UPPAAL. Both these approaches are in principle prone to a $2^{\#\mathcal{D}}$ blowup compared to the first approach, where $\#\mathcal{D}$ gives the number of diagonal constraints. The table shows that a good extent of this blowup indeed happens. The UPPAAL diagonal free engine uses "minimal constraint systems" [6] for representing zones, whereas TChecker uses DBMs [15]. This explains why even with the same number of nodes visited, UPPAAL performs better in terms of time. We have not included in the table the comparison with two other works dealing with the same problem: the refined diagonal free conversion [30] and the extension of LU simulation for diagonals [18]. However, our results are better than the tables reported in these papers.

7 Conclusion

We have proposed a new algorithm for handling diagonal constraints in timed automata, and extended it to automata with general updates. Our approach is based on a simulation relation between zones. From our preliminary experiments, we can infer that the use of simulations is indispensable in the presence of diagonal constraints as zone-splitting can be avoided. Moreover, the fact that the simulation approach stores the actual zones (as opposed to abstracted zones in the extrapolation approach) has enabled optimizations for diagonal-free automata that work with dynamically changing simulation parameters (LU-bounds), which are learnt as and when the zones are expanded [22]. Working with actual zones is also convenient for finding cost-optimal paths in priced timed automata [11]. Investigating these in the presence of diagonal constraints is part of future work. Currently, we have not implemented our approach for updateable timed automata. This will also be part of our future work.

Working directly with a model containing diagonal constraints could be convenient (both during modeling, and during extraction of diagnostic traces) and can also potentially give a smaller automaton to begin with. We believe that our experiments provide hope that diagonal constraints can indeed be used.

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Safety and Co-safety Comparator Automata for Discounted-Sum Inclusion

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Abstract. *Discounted-sum inclusion* (DS-inclusion, in short) formalizes the goal of comparing quantitative dimensions of systems such as cost, resource consumption, and the like, when the mode of aggregation for the quantitative dimension is discounted-sum aggregation. *Discounted-sum comparator automata*, or *DS-comparators* in short, are Büchi automata that read two infinite sequences of weights synchronously and relate their discounted-sum. Recent empirical investigations have shown that while DS-comparators enable competitive algorithms for DS-inclusion, they still suffer from the scalability bottleneck of Büchi operations.

Motivated by the connections between discounted-sum and Büchi automata, this paper undertakes an investigation of language-theoretic properties of DS-comparators in order to mitigate the challenges of Büchi DS-comparators to achieve improved scalability of DS-inclusion. Our investigation uncovers that DS-comparators possess safety and co-safety language-theoretic properties. As a result, they enable reductions based on subset construction-based methods as opposed to higher complexity Büchi complementation, yielding tighter worst-case complexity and improved empirical scalability for DS-inclusion.

1 Introduction

The analysis of quantitative dimensions of computing systems such as cost, resource consumption, and distance metrics [6,10,28] has been studied thoroughly to design efficient computing systems. Cost-aware program-synthesis [14,16] and low-cost program-repair [25] have found compelling applications in robotics [24,29], education [22], and the like. *Quantitative verification* facilitates efficient system design by automatically determining if a system implementation is more efficient than a specification model. Investigations in quantitative verification have demonstrated their high computational complexity and practically intractable [17,23]. This work addresses practical intractability of quantitative verification.

At the core of quantitative verification lies the problem of *quantitative inclusion* which formalizes the goal of determining which of two given systems is more efficient [17,23,31]. In quantitative inclusion, quantitative systems are abstracted as weighted automata [7,21,32]. A run in a weighted automaton is associated with a sequence of weights. The quantitative dimension of these runs is determined by the weight of runs, which is computed by taking an aggregate of the

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run's weight sequence. Quantitative inclusion can be thought of as the quantitative generalization of (qualitative) language inclusion.

A commonly appearing mode of aggregation is that of *Discounted-sum (DS) aggregation* which captures the intuition that weights incurred in the near future are more significant than those incurred later on [19]. The convergence of DS aggregation for all bounded infinite weight-sequences makes it a preferred mode of aggregation across domains: Reinforcement learning [37], planning under uncertainty [34], and game-theory [33]. This work examines the problem of *Discounted-sum inclusion* or *DS-inclusion* that is quantitative inclusion when *discounted sum* is the mode of aggregation.

In theory, DS-inclusion is PSPACE-complete [12]. Recent algorithmic approaches have tapped into language-theoretic properties of discounted-sum aggregate function [12,18] to design practical algorithms for DS-inclusion [11,12]. These algorithms use *DS-comparator automata* (*DS-comparator*, in short) as their main technique, and are *purely* automata-theoretic. While these algorithms outperform other existing approaches for DS-inclusion in runtime [15,17], even these do not scale well on weighted-automata with more than few hundreds of states [11]. This work contributes novel techniques and algorithms for DS-inclusion to address the scalability challenge of DS-inclusion

An in-depth examination of the DS-comparator based algorithm exposes their scalability bottleneck. DS-comparator is a Büchi automaton that relates the discounted-sum aggregate of two (bounded) weight-sequences A and B by determining the membership of the interleaved pair of sequences (A, B) in the language of the comparator. As a result, DS-comparators reduce DS-inclusion to language inclusion between (non-deterministic) Büchi automaton. In spite of the fact that many techniques have been proposed to solve Büchi language inclusion efficiently in practice [4,20], none of them can avoid at least an exponential blow-up of $2^{\mathcal{O}(n \log n)}$, for an n-sized input, caused by a direct or indirect involvement of Büchi complementation [36,40].

This work meets the scalability challenge of DS-inclusion by delving deeper into language-theoretic properties of discounted-sum aggregate functions [18] in order to obtain algorithms for DS-inclusion that render both tighter theoretical complexity and improved scalability. Specifically, we prove that DS-comparators are expressed as *safety automata* or *co-safety automata* [26] (Sect. 3.1), and have compact deterministic constructions (Sect. 3.2). Safety and co-safety automata have the property that their complementation is performed by simpler and lower $2^{\mathcal{O}(n)}$-complexity subset-construction methods [27]. As a result, they facilitate a procedure for DS-inclusion that uses subset-construction based intermediate steps instead of Büchi complementation, yielding an improvement in theoretical complexity from $2^{\mathcal{O}(n \cdot \log n)}$ to $2^{\mathcal{O}(n)}$. Our subset-construction based procedure has yet another advantage over Büchi complementation as they support efficient on-the-fly implementations, yielding practical scalability as well (Sect. 4).

An empirical evaluation of our prototype tool QuIPFly for the proposed procedure against the prior DS-comparator algorithm and other existing approaches for DS-inclusion shows that QuIPFly outperforms them by orders of magnitude both in runtime and the number of benchmarks solved (Sect. 4).

2 Preliminaries and Related Work

A weight-sequence, finite or infinite, is *bounded* if the absolute value of all of its elements are bounded by a fixed number.

Büchi Automaton: A *Büchi automaton* is a tuple $\mathcal{A} = (S, \Sigma, \delta, s_{\mathcal{I}}, \mathcal{F})$, where S is a finite set of *states*, Σ is a finite *input alphabet*, $\delta \subseteq (S \times \Sigma \times S)$ is the *transition relation*, state $s_{\mathcal{I}} \in S$ is the *initial state*, and $\mathcal{F} \subseteq S$ is the set of *accepting states* [39]. A Büchi automaton is *deterministic* if for all states s and inputs a, $|\{s' | (s, a, s') \in \delta \text{ for some } s'\}| \leq 1$. Otherwise, it is *nondeterministic*. A Büchi automaton is *complete* if for all states s and inputs a, $|\{s' | (s, a, s') \in \delta \text{ for some } s'\}| \geq 1$. For a word $w = w_0 w_1 \cdots \in \Sigma^\omega$, a *run* ρ of w is a sequence of states $s_0 s_1 \ldots$ s.t. $s_0 = s_{\mathcal{I}}$, and $\tau_i = (s_i, w_i, s_{i+1}) \in \delta$ for all i. Let $inf(\rho)$ denote the set of states that occur infinitely often in run ρ. A run ρ is an *accepting run* if $inf(\rho) \cap \mathcal{F} \neq \emptyset$. A word w is an accepting word if it has an accepting run. The language of Büchi automaton $\mathcal{A}$, denoted by $\mathcal{L}(\mathcal{A})$ is the set of all words accepted by $\mathcal{A}$. By abuse of notation, we write $w \in \mathcal{A}$ and $\rho \in \mathcal{A}$ if w and ρ are an accepting word and an accepting run of $\mathcal{A}$. Büchi automata are closed under set-theoretic union, intersection, and complementation [39].

Safety and Co-safety Properties: Let $\mathcal{L} \subseteq \Sigma^\omega$ be a language over alphabet Σ. A finite word $w \in \Sigma^*$ is a *bad prefix* for $\mathcal{L}$ if for all infinite words $y \in \Sigma^\omega$, $x \cdot y \notin \mathcal{L}$. A language $\mathcal{L}$ is a *safety language* if every word $w \notin \mathcal{L}$ has a bad prefix for $\mathcal{L}$. A language $\mathcal{L}$ is a *co-safety language* if its complement language is a safety language [5]. When a safety or co-safety language is an ω-regular language, the Büchi automaton representing it is called a safety or co-safety automaton, respectively [26]. Wlog, safety and co-safety automaton contain a *sink state* from which every outgoing transitions loops back to the sink state and there is a transition on every alphabet symbol. All states except the sink state are accepting in a safety automaton, while only the sink state is accepting in a co-safety automaton. Unlike Büchi complementation, complementation of safety and co-safety automaton is conducted by simpler subset construction with a lower $2^{\mathcal{O}(n)}$ blow-up. The complementation of safety automaton is a co-safety automaton, and vice-versa. Safety automata are closed under intersection, and co-safety automata are closed under union.

Comparator Automaton: For a finite-set of integers Σ, an aggregate function $f : \mathbb{Z}^\omega \to \mathbb{R}$, and equality or inequality relation $\mathsf{R} \in \{<, >, \leq, \geq, =, \neq\}$, the *comparison language for f with relation* R is a language of infinite words over the alphabet $\Sigma \times \Sigma$ that accepts a pair (A, B) iff $f(A)\ \mathsf{R}\ f(B)$ holds. A *comparator automaton (comparator, in short) for aggregate function f and relation* R is an automaton that accepts the comparison language for f with R [12]. A comparator is said to be *regular* if its automaton is a Büchi automaton.

Weighted Automaton: A *weighted automaton* over infinite words is a tuple $\mathcal{A} = (\mathcal{M}, \gamma, f)$, where $\mathcal{M} = (S, \Sigma, \delta, s_{\mathcal{I}}, S)$ is a complete Büchi automaton

with all states as accepting, $\gamma : \delta \to \mathbb{N}$ is a *weight function*, and $f : \mathbb{N}^\omega \to \mathbb{R}$ is the *aggregate function* [17,31]. *Words* and *runs* in weighted automata are defined as in Büchi automata. The *weight-sequence* of run $\rho = s_0 s_1 \dots$ of word $w = w_0 w_1 \dots$ is given by $wt_\rho = n_0 n_1 n_2 \dots$ where $n_i = \gamma(s_i, w_i, s_{i+1})$ for all i. The *weight of a run* ρ, denoted by $f(\rho)$, is given by $f(wt_\rho)$. Here the *weight of a word* $w \in \Sigma^\omega$ in weighted automata is defined as $wt_{\mathcal{A}}(w) = sup\{f(\rho) | \rho$ is a run of w in $\mathcal{A}\}$.

Quantitative Inclusion: Let P and Q be weighted automata with the *same* aggregate function. The *strict quantitative inclusion problem*, denoted by $P \subset Q$, asks whether for all words $w \in \Sigma^\omega$, $wt_P(w) < wt_Q(w)$. The *non-strict quantitative inclusion problem*, denoted by $P \subseteq Q$, asks whether for all words $w \in \Sigma^\omega$, $wt_P(w) \leq wt_Q(w)$. *Comparison language or comparator of a quantitative inclusion* problem refer to the comparison language or comparator of the associated aggregate function.

Discounted-sum Inclusion: Let $A = A_0, A_1, \dots$ be a weight sequence, $d > 1$ be a rational number. The *discounted-sum* (DS in short) of A with *integer* discount-factor $d > 1$ is $DS(A, d) = \Sigma_{i=0}^{\infty} \frac{A_i}{d^i}$. DS-comparison language and DS-comparator with discount-factor $d > 1$ are the comparison language and comparator obtained for the discounted-sum aggregate function with discount-factor $d > 1$, respectively. Strict or non-strict discounted-sum inclusion is strict or non-strict quantitative inclusion with the discounted-sum aggregate function, respectively. For brevity, we abbreviate discounted-sum inclusion to DS-inclusion.

Related Work. The decidability of DS-inclusion is an open problem when the discount-factor $d > 1$ is arbitrary. Recent work has established that DS-inclusion is PSPACE-complete when the discount-factor is an integer [12]. This work investigates algorithmic approaches to DS-inclusion with integer discount-factors.

Two contrasting solution approaches have been identified for DS-inclusion. The first approach is *hybrid* [17]. It separates out the language-theoretic aspects of weighted-automata from the numerical aspects, and solves each separately [15,17]. More specifically, the hybrid approach solves the language-theoretic aspects by DS-determinization [15] and the numerical aspect is performed by linear programming [8,9] sequentially. To the best of our knowledge, this procedure cannot be performed in parallel. As a result, this approach must always incur the exponential cost of DS-determinization.

The second approach is *purely*-automata theoretic [12]. This approach uses regular DS-comparator to reduce DS-inclusion to language inclusion between nondeterministic Büchi automata [11,12]. While the purely automata-theoretic approach scales better than the hybrid approach in runtime [11], its scalability suffers from fundamental algorithmic limitations of Büchi language inclusion. A key ingredient of Büchi language-inclusion is Büchi complementation [36]. Büchi complementation is $2^{\mathcal{O}(n \log n)}$ in the worst-case, and is practically intractable [40]. These limitations also feature in the theoretical complexity and practical performance of DS-inclusion. The complexity of DS-inclusion between weighted

automata P and Q with regular DS-comparator C for integer discount-factor $d > 1$ is $|P| \cdot 2^{\mathcal{O}(|P||Q||C| \cdot \log(|P||Q||C|))}$.

This work improves the worst-case complexity and practical performance of the purely automata theoretic approach for DS-inclusion by a closer investigation of language-theoretic properties of DS-comparators. In particular, we identify that DS-comparator for integer discount-factor form a safety or co-safety automata (depending on the relation R). We show that complementation advantage of safety/co-safety automata not only improves the theoretical complexity of DS-inclusion with integer discount-factor but also facilitate on-the-fly implementations that significantly improve practical performance.

3 DS-inclusion with Integer Discount-Factor

This section covers the core technical contributions of this paper. We uncover novel language-theoretic properties of DS-comparison languages and utilize them to obtain tighter theoretical upper-bound for DS-inclusion with integer discount-factor. Unless mentioned otherwise, the discount-factor is an integer.

In Sect. 3.1 we prove that DS-comparison languages are either safety or co-safety for all rational discount-factors. Since DS-comparison languages are ω-regular for integer discount-factors [12], we obtain that DS-comparators for integer discount-factors form safety or co-safety automata. Next, Sect. 3.2 makes use of newly obtained safety/co-safety properties of DS-comparator to present the first deterministic constructions for DS-comparators. These deterministic construction are compact in the sense that they match their non-deterministic counterparts in number of states [11]. Section 3.3 evaluates the complexity of quantitative inclusion with regular safety/co-safety comparators, and observes that its complexity is lower than the complexity for quantitative inclusion with regular comparators. Finally, since DS-comparators are regular safety/co-safety, our analysis shows that the complexity of DS-inclusion is improved as a consequence of the complexity observed for quantitative-inclusion with regular safety/co-safety comparators.

We begin with formal definitions of safety/co-safety comparison languages and safety/co-safety comparators:

Definition 1 (Safety and co-safety comparison languages). *Let Σ be a finite set of integers, $f : \mathbb{Z}^\omega \to \mathbb{R}$ be an aggregate function, and $\mathsf{R} \in \{\leq, <, \geq, >, =, \neq\}$ be a relation. A comparison language L over $\Sigma \times \Sigma$ for aggregate function f and relation R is said to be a safety comparison language (or a co-safety comparison language) if L is a safety language (or a co-safety language).*

Definition 2 (Safety and co-safety comparators). *Let Σ be a finite set of integers, $f : \mathbb{Z}^\omega \to \mathbb{R}$ be an aggregate function, and $\mathsf{R} \in \{\leq, <, \geq, >, =, \neq\}$ be a relation. A comparator for aggregate function f and relation R is a* safety comparator *(or* co-safety comparator*) is the comparison language for f and R is a safety language (or co-safety language).*

A safety comparator is *regular* if its language is ω-regular (equivalently, if its automaton is a safety automaton). Likewise, a co-safety comparator is *regular* if its language is ω-regular (equivalently, automaton is a co-safety automaton).

By complementation duality of safety and co-safety languages, comparison language for an aggregate function f for non-strict inequality $\leq$ is safety iff the comparison language for f for strict inequality $<$ is co-safety. Since safety languages and safety automata are closed under intersection, safety comparison languages and regular safety comparator for non-strict inequality renders the same for equality. Similarly, since co-safety languages and co-safety automata are closed under union, co-safety comparison languages and regular co-safety comparators for non-strict inequality render the same for the inequality relation. Therefore, it suffices to examine the comparison language for one relation only.

It is worth noting that for weight-sequences A and B and all relations R, we have that $DS(A,d)\ \mathsf{R}\ DS(B,d)$ iff $DS(A-B,d)\ \mathsf{R}\ 0$, where $(A-B)_i = A_i - B_i$ for all $i \geq 0$. Prior work [11] shows that we can define *DS-comparison language* with upper bound μ, discount-factor $d > 1$, and relation R to accept infinite and bounded weight-sequence C over $\{-\mu, \ldots, \mu\}$ iff $DS(C,d)\ \mathsf{R}\ 0$ holds. Similarly, DS-comparator with the same parameters μ, $d > 1$, accepts the DS-comparison language with parameters μ, d and R. We adopt these definitions for DS-comparison languages and DS-comparators

Throughout this section, the concatenation of finite sequence x with finite or infinite sequence y is denoted by $x \cdot y$ in the following.

3.1 DS-comparison Languages and Their Safety/Co-safety Properties

The central result of this section is that DS-comparison languages are safety or co-safety languages for all (integer and non-integer) discount-factors (Theorem 1). In particular, since DS-comparison languages are ω-regular for integer discount-factors [12], this implies that DS-comparators for integer discount-factors form safety or co-safety automata (Corollary 1).

The argument for safety/co-safety of DS-comparison languages depends on the property that the discounted-sum aggregate of all bounded weight-sequences exists for all discount-factors $d > 1$ [35].

Theorem 1. *Let $\mu > 1$ be the upper bound. For rational discount-factor $d > 1$*

1. *DS-comparison languages are safety languages for relations $\mathsf{R} \in \{\leq, \geq, =\}$*
2. *DS-comparison language are co-safety languages for relations $\mathsf{R} \in \{<, >, \neq\}$.*

Proof (Proof sketch). Due to duality of safety/co-safety languages, it suffices to show that DS-comparison language with $\leq$ is a safety language.

Let DS-comparison language with upper bound μ, rational discount-factor $d > 1$ and relation $\leq$ be denoted by $\mathcal{L}_{\leq}^{\mu,d}$. Suppose that $\mathcal{L}_{\leq}^{\mu,d}$ is not a safety language. Let W be a weight-sequence in the complement of $\mathcal{L}_{\leq}^{\mu,d}$ such that W does not have a bad prefix. Then the following hold: (a). $DS(W,d) > 0$ (b).

For all $i \geq 0$, the i-length prefix $W[i]$ of W can be extended to an infinite and bounded weight-sequence $W[i] \cdot Y^i$ such that $DS(W[i] \cdot Y^i, d) \leq 0$.

Note that $DS(W, d) = DS(W[i], d) + \frac{1}{d^i} \cdot DS(W[i \ldots], d)$ where $W[i \ldots] = W_i W_{i+1} \ldots$ and $DS(W[i], d)$ is the discounted-sum of the finite sequence $W[i]$ i.e. $DS(W[i], d) = \Sigma_{j=0}^{j=i-1} \frac{W[j]}{d^j}$. Similarly, $DS(W[i] \cdot Y^i, d) = DS(W[i], d) + \frac{1}{d^i} \cdot DS(Y^i, d)$. The contribution of tail sequences $W[i \ldots]$ and Y^i to the discounted-sum of W and $W[i] \cdot Y^i$, respectively, diminishes exponentially as the value of i increases. In addition, since W and $W[i] \cdot Y^i$ share a common i-length prefix $W[i]$, their discounted-sum values must converge to each other. The discounted sum of W is fixed and greater than 0, due to convergence there must be a $k \geq 0$ such that $DS(W[k] \cdot Y^k, d) > 0$. Contradiction to (b).

Therefore, DS-comparison language with $\leq$ is a safety language. □

Semantically this result implies that for a bounded-weight sequence C and rational discount-factor $d > 1$, if $DS(C, d) > 0$ then C must have a finite prefix C_{pre} such that the discounted-sum of the finite prefix is so large that no infinite extension by bounded weight-sequence Y can reduce the discounted-sum of $C_{\mathsf{pre}} \cdot Y$ with the same discount-factor d to zero or below.

Prior work shows that DS-comparison languages are expressed by Büchi automata iff the discount-factor is an integer [13]. Therefore:

Corollary 1. *Let $\mu > 1$ be the upper bound. For* integer *discount-factor $d > 1$*

1. *DS-comparators are regular safety for relations* $\mathsf{R} \in \{\leq, \geq, =\}$
2. *DS-comparators are regular co-safety for relations* $\mathsf{R} \in \{<, >, \neq\}$.

Lastly, it is worth mentioning that for the same reason [13] DS-comparators for non-integer rational discount-factors do not form safety or co-safety automata.

3.2 Deterministic DS-comparator for Integer Discount-Factor

This section issues deterministic safety/co-safety constructions for DS-comparators with integer discount-factors. This is different from prior works since they supply non-deterministic Büchi constructions only [11,12]. An outcome of DS-comparators being regular safety/co-safety (Corollary 1) is a proof that DS-comparators permit deterministic Büchi constructions, since non-deterministic and deterministic safety automata (and co-safety automata) have equal expressiveness [26]. Therefore, one way to obtain deterministic Büchi construction for DS-comparators is to determinize the non-deterministic constructions using standard procedures [26,36]. However, this will result in exponentially larger deterministic constructions. To this end, this section offers direct deterministic safety/co-safety automata constructions for DS-comparator that not only avoid an exponential blow-up but also match their non-deterministic counterparts in number of states (Theorem 3).

Key ideas. Due to duality and closure properties of safety/co-safety automata, we only present the construction of deterministic safety automata for DS-comparator with upper bound μ, integer discount-factor $d > 1$ and relation $\leq$, denoted by $\mathcal{A}^{\mu,d}_{\leq}$. We proceed by obtaining a *deterministic finite automaton*, (DFA), denoted by $\mathsf{bad}(\mu, d, \leq)$, for the language of bad-prefixes of $\mathcal{A}^{\mu,d}_{\leq}$ (Theorem 2). Trivial modifications to $\mathsf{bad}(\mu, d, \leq)$ will furnish the coveted deterministic safety automata for $\mathcal{A}^{\mu,d}_{\leq}$ (Theorem 3).

Construction. We begin with some definitions. Let W be a *finite* weight-sequence. By abuse of notation, the discounted-sum of finite-sequence W with discount-factor d is defined as $DS(W, d) = DS(W \cdot 0^{\omega}, d)$. The *recoverable-gap* of a finite weight-sequences W with discount factor d, denoted $\mathsf{gap}(W, d)$, is its normalized discounted-sum: If $W = \varepsilon$ (the empty sequence), $\mathsf{gap}(\varepsilon, d) = 0$, and $\mathsf{gap}(W, d) = d^{|W|-1} \cdot DS(W, d)$ otherwise [15]. Observe that the recoverable-gap has an inductive definition i.e. $\mathsf{gap}(\varepsilon, d) = 0$, where ε is the empty weight-sequence, and $\mathsf{gap}(W \cdot v, d) = d \cdot \mathsf{gap}(W, d) + v$, where $v \in \{-\mu, \ldots, \mu\}$.

This observation influences a sketch for $\mathsf{bad}(\mu, d, \leq)$. Suppose all possible values for recoverable-gap of weight sequences forms the set of states. Then, the transition relation of the DFA can mimic the inductive definition of recoverable gap i.e. there is a transition from state s to t on alphabet $v \in \{-\mu, \ldots, \mu\}$ iff $t = d \cdot s + v$, where s and v are recoverable-gap values of weight-sequences. There is one caveat here: There are infinitely many possibilities for the values of recoverable gap. We need to limit the recoverable gap values to finitely many values of interest. The core aspect of this construction is to identify these values.

First, we obtain a lower bound on recoverable gap for bad-prefixes of $\mathcal{A}^{\mu,d}_{\leq}$:

Lemma 1. *Let μ and $d > 1$ be the bound and discount-factor, resp. Let $\mathsf{T} = \frac{\mu}{d-1}$ be the threshold value. Let W be a non-empty, bounded, finite weight-sequence. Weight sequence W is a bad-prefix of $\mathcal{A}^{\mu,d}_{\leq}$ iff $\mathsf{gap}(W, d) > \mathsf{T}$.*

Proof. Let a finite weight-sequence W be a bad-prefix of $\mathcal{A}^{\mu,d}_{\leq}$. Then, $DS(W \cdot Y, d) > 0$ for all infinite and bounded weight-sequences Y. Since $DS(W \cdot Y, d) = DS(W, d) + \frac{1}{d^{|W|}} \cdot DS(Y, d)$, we get $\inf(DS(W, d) + \frac{1}{d^{|W|}} \cdot DS(Y, d)) > 0 \implies DS(W, d) + + \frac{1}{d^{|W|}} \cdot \inf(DS(Y, d)) > 0$ as W is a fixed sequence. Hence $DS(W, d) + \frac{-\mathsf{T}}{d^{|W|-1}} > 0 \implies \mathsf{gap}(W, d) - T > 0$. Conversely, for all infinite, bounded, weight-sequence Y, $DS(W \cdot Y, d) \cdot d^{|W|-1} = \mathsf{gap}(W, d) + \frac{1}{d} \cdot DS(Y, d)$. Since $\mathsf{gap}(W, d) > T$, $\inf(DS(Y, d)) = -\mathsf{T} \cdot d$, we get $DS(W \cdot Y, d) > 0$. □

Since all finite and bounded extensions of bad-prefixes are also bad-prefixes, Lemma 1 implies that if the recoverable-gap of a finite sequence is strinctly lower that threshold T, then recoverable gap of all of its extensions also exceed T. Since recoverable gap exceeding threshold T is the precise condition for bad-prefixes, all states with recoverable gap exceeding T can be merged into a single state. Note, this state forms an accepting sink in $\mathsf{bad}(\mu, d, \leq)$.

Next, we attempt to merge very low recoverable gap value into a single state. For this purpose, we define *very-good prefixes* for $\mathcal{A}^{\mu,d}_{\leq}$: A finite and bounded weight-sequence W is a *very good* prefix for language of $\mathcal{A}^{\mu,d}_{\leq}$ if for all infinite, bounded extensions of W by Y, $DS(W \cdot Y, d) \leq 0$. A proof similar to Lemma 1 proves an upper bound for the recoverable gap of very-good prefixes of $\mathcal{A}^{\mu,d}_{\leq}$:

Lemma 2. *Let μ and $d > 1$ be the bound and discount-factor, resp. Let $\mathsf{T} = \frac{\mu}{d-1}$ be the threshold value. Let W be a non-empty, bounded, finite weight-sequence. Weight-sequence W is a very-good prefix of $\mathcal{A}^{\mu,d}_{\leq}$ iff $\mathsf{gap}(W, d) \leq -\mathsf{T}$.*

Clearly, finite extensions of very-good prefixes are also very-good prefixes. Further, $\mathsf{bad}(\mu, d, \leq)$ must not accept very-good prefixes. Thus, by reasoning as earlier we get that all recoverable gap values that are less than or equal to $-\mathsf{T}$ can be merged into one non-accepting sink state in $\mathsf{bad}(\mu, d, \leq)$.

Finally, for an integer discount-factor the recoverable gap is an integer. Let $\lfloor x \rfloor$ denote the floor of $x \in \mathbb{R}$ e.g. $\lfloor 2.3 \rfloor = 2$, $\lfloor -2 \rfloor = -2$, $\lfloor -2.3 \rfloor = -3$. Then,

Corollary 2. *Let μ be the bound and $d > 1$ an integer discount-factor. Let $\mathsf{T} = \frac{\mu}{d-1}$ be the threshold. Let W be a non-empty, bounded, finite weight-sequence.*

- *W is a bad prefix of $\mathcal{A}^{\mu,d}_{\leq}$ iff $\mathsf{gap}(W, d) > \lfloor \mathsf{T} \rfloor$*
- *W is a very-good prefix of $\mathcal{A}^{\mu,d}_{\leq}$ iff $\mathsf{gap}(W, d) \leq \lfloor -\mathsf{T} \rfloor$*

So, the recoverable gap value is either one of $\{\lfloor -\mathsf{T} \rfloor + 1, \ldots, \lfloor \mathsf{T} \rfloor\}$, or less than or equal to $\lfloor -\mathsf{T} \rfloor$, or greater than $\lfloor \mathsf{T} \rfloor$. This curbs the state-space to $\mathcal{O}(\mu)$-many values of interest, as $\mathsf{T} = \frac{\mu}{d-1} < \frac{\mu \cdot d}{d-1}$ and $1 < \frac{d}{d-1} \leq 2$. Lastly, since $\mathsf{gap}(\varepsilon, d) = 0$, state 0 must be the initial state.

Construction of $\mathsf{bad}(\mu, d, \leq)$. Let μ be the upper bound, and $d > 1$ be the integer discount-factor. Let $\mathsf{T} = \frac{\mu}{d-1}$ be the threshold value. The finite-state automata $\mathsf{bad}(\mu, d, \leq) = (S, s_I, \Sigma, \delta, \mathcal{F})$ is defined as follows:

- States $S = \{\lfloor -\mathsf{T} \rfloor + 1, \ldots, \lfloor \mathsf{T} \rfloor\} \cup \{\mathsf{bad}, \mathsf{veryGood}\}$
- Initial state $s_I = 0$, Accepting states $\mathcal{F} = \{\mathsf{bad}\}$
- Alphabet $\Sigma = \{-\mu, -\mu + 1, \ldots, \mu - 1, \mu\}$
- Transition function $\delta \subseteq S \times \Sigma \to S$ where $(s, a, t) \in \delta$ then:
  1. If $s \in \{\mathsf{bad}, \mathsf{veryGood}\}$, then $t = s$ for all $a \in \Sigma$
  2. If $s \in \{\lfloor -\mathsf{T} \rfloor + 1, \ldots, \lfloor \mathsf{T} \rfloor\}$, and $a \in \Sigma$
     (a) If $\lfloor -\mathsf{T} \rfloor < d \cdot s + a \leq \lfloor \mathsf{T} \rfloor$, then $t = d \cdot s + a$
     (b) If $d \cdot s + a > \lfloor \mathsf{T} \rfloor$, then $t = \mathsf{bad}$
     (c) If $d \cdot s + a \leq \lfloor -\mathsf{T} \rfloor$, then $t = \mathsf{veryGood}$

Theorem 2. *Let μ be the upper bound, $d > 1$ be the integer discount-factor. $\mathsf{bad}(\mu, d, \leq)$ accepts finite, bounded, weight-sequence iff it is a bad-prefix of $\mathcal{A}^{\mu,d}_{\leq}$.*

Proof (Proof sketch). First note that the transition relation is deterministic and complete. Therefore, every word has a unique run in $\mathsf{bad}(\mu, d, \leq)$. Let last be

the last state in the run of finite, bounded, weight-sequence W in the DFA. Use induction on the length of W to prove the following:

- $\mathsf{last} \in \{\lfloor -\mathsf{T} \rfloor + 1, \ldots, \lfloor \mathsf{T} \rfloor\}$ iff $\mathsf{gap}(W, d) = \mathsf{last}$
- $\mathsf{last} = \mathsf{bad}$ iff $\mathsf{gap}(W, d) > \lfloor \mathsf{T} \rfloor$
- $\mathsf{last} = \mathsf{veryGood}$ iff $\mathsf{gap}(W, d) \leq \lfloor -\mathsf{T} \rfloor$

Therefore, a finite, bounded weight-sequence is accepted iff its recoverable gap is greater than $\lfloor \mathsf{T} \rfloor$. In other words, iff it is a bad-prefix of $\mathcal{A}_{\leq}^{\mu,d}$. □

$\mathcal{A}_{\leq}^{\mu,d}$ is obtained from $\mathsf{bad}(\mu, d, \leq)$ by applying co-Büchi acceptance condition.

Theorem 3. *Let μ be the upper bound, and $d > 1$ be the integer discount-factor. DS-comparator for all inequalities and equality are either deterministic safety or deterministic co-safety automata with $\mathcal{O}(\mu)$ states.*

As a matter of fact, the most compact non-deterministic DS-comparator constructions with parameters μ, d and R also contain $\mathcal{O}(\mu)$ states [11].

3.3 Quantitative Inclusion with Safety/Co-safety Comparators

This section investigates quantitative language inclusion with regular safety/co-safety comparators. Unlike quantitative inclusion with regular comparators, quantitative inclusion with regular safety/co-safety comparators is able to circumvent Büchi complementation with intermediate subset-construction steps. As a result, complexity of quantitative inclusion with regular safety/co-safety comparator is lower than the same with regular comparators [12] (Theorem 4). Finally, since DS-comparators are regular safety/co-safety comparators, the algorithm for quantitative inclusion with regular safety/co-safety comparators applies to DS-inclusion yielding a lower complexity algorithm for DS-inclusion (Corollary 5).

Key Ideas A run of word w in a weighted-automaton is *maximal* if its weight is the supremum weight of all runs of w in the weighted-automaton. A run ρ_P of w in P is a *counterexample* for $P \subseteq Q$ (or $P \subset Q$) iff there exists a maximal run sup_Q of w in Q such that $wt(\rho_P) > wt(sup_Q)$ (or $wt(\rho_P) \geq wt(sup_Q)$). Consequently, $P \subseteq Q$ (or $P \subset Q$) iff there are no counterexample runs in P. Therefore, the roadmap to solve quantitative inclusion for regular safety/co-safety comparators is as follows:

1. Use regular safety/co-safety comparators to construct the *maximal automaton* of Q i.e. an automaton that accepts all maximal runs of Q (Corollary 3).
2. Use the regular safety/co-safety comparator and the maximal automaton to construct a *counterexample automaton* that accepts all counterexample runs of the inclusion problem $P \subseteq Q$ (or $P \subset Q$) (Lemma 5).

3. Solve quantitative inclusion for safety/co-safety comparator by checking for emptiness of the counterexample (Theorem 4).
   Finally, since DS-comparators are regular safety/co-safety automaton (Corollary 1), apply Theorem 4 to obtain an algorithm for DS-inclusion that uses regular safety/co-safety comparators (Corollary 5).

Let W be a weighted automaton. Then the *annotated automaton* of W, denoted by $\hat{W}$, is the Büchi automaton obtained by transforming transition $s \xrightarrow{a} t$ with weight v in W to transition $s \xrightarrow{a,v} t$ in $\hat{W}$. Observe that $\hat{W}$ is a safety automaton since all its states are accepting. A run on word w with weight sequence wt in W corresponds to an *annotated word* (w, wt) in $\hat{W}$, and vice-versa.

Maximal Automaton. This section covers the construction of the *maximal automaton* from a weighted automaton. Let W and $\hat{W}$ be a weighted automaton and its annotated automaton, respectively. We call an annotated word (w, wt_1) in $\hat{W}$ *maximal* if for all other words of the form (w, wt_2) in $\hat{W}$, $wt(wt_1) \geq wt(wt_2)$. Clearly, (w, wt_1) is a maximal word in $\hat{W}$ iff word w has a run with weight sequence wt_1 in W that is maximal. We define *maximal automaton* of weighted automaton W, denoted $\mathsf{Maximal}(W)$, to be the automaton that accepts all maximal words of its annotated automata $\hat{W}$.

We show that when the comparator is regular safety/co-safety, the construction of the maximal automata incurs a $2^{\mathcal{O}(n)}$ blow-up. This section exposes the construction for maximal automaton when comparator for non-strict inequality is regular safety. The other case when the comparator for strict inequality is regular co-safety has been deferred to the appendix.

Lemma 3. *Let W be a weighted automaton with regular safety comparator for non-strict inequality. Then the language of* $\mathsf{Maximal}(W)$ *is a safety language.*

Proof (Proof sketch). An annotated word (w, wt_1) is not maximal in $\hat{W}$ for one of the following two reasons: Either (w, wt_1) is not a word in $\hat{W}$, or there exists another word (w, wt_2) in $\hat{W}$ s.t. $wt(wt_1) < wt(wt_2)$ (equivalently (wt_1, wt_2) is not in the comparator non-strict inequality). Both $\hat{W}$ and comparator for non-strict inequality are safety languages, so the language of maximal words must also be a safety language. □

We now proceed to construct the safety automata for $\mathsf{Maximal}(W)$

Intuition. The intuition behind the construction of maximal automaton follows directly from the definition of maximal words. Let $\hat{W}$ be the annotated automaton for weighted automaton W. Let $\hat{\Sigma}$ denote the alphabet of $\hat{W}$. Then an annotated word $(w, wt_1) \in \hat{\Sigma}^\omega$ is a word in $\mathsf{Maximal}(W)$ if (a) $(w, wt_1) \in \hat{W}$, and (b) For all words $(w, wt_2) \in \hat{W}$, $wt(wt_1) \geq wt(wt_2)$.

The challenge here is to construct an automaton for condition (b). Intuitively, this automaton simulates the following action: As the automaton reads word (w, wt_1), it must spawn all words of the form (w, wt_2) in $\hat{W}$, while also ensuring that $wt(wt_1) \geq wt(wt_2)$ holds for every word (w, wt_2) in $\hat{W}$. Since $\hat{W}$ is a safety

automaton, for a word $(w, wt_1) \in \hat{\Sigma}^\omega$, all words of the form $(w, wt_2) \in \hat{W}$ can be traced by subset-construction. Similarly since the comparator C for non-strict inequality ($\geq$) is a safety automaton, all words of the form $(wt_1, wt_2) \in C$ can be traced by subset-construction as well. The construction needs to carefully align the word (w, wt_1) with the all possible $(w, wt_2) \in \hat{W}$ and $(wt_1, wt_2) \in C$.

Construction of $\mathsf{Maximal}(W)$. Let W be a weighted automaton, with annotated automaton $\hat{W}$ and C denote its regular safety comparator for non-strict inequality. Let S_W denote the set of states of W (and $\hat{W}$) and S_C denote the set of states of C. We define $\mathsf{Maximal}(W) = (S, s_I, \hat{\Sigma}, \delta, \mathcal{F})$ as follows:

- Set of states S consists of tuples of the form (s, X), where $s \in S_W$, and $X = \{(t, c) | t \in S_W, c \in S_C\}$
- $\hat{\Sigma}$ is the alphabet of $\hat{W}$
- Initial state $s_I = (s_w, \{(s_w, s_c)\})$, where s_w and s_c are initial states in $\hat{W}$ and C, respectively.
- Let states $(s, X), (s, X') \in S$ such that $X = \{(t_1, c_1), \ldots, (t_n, c_n)\}$ and $X' = \{(t'_1, c'_1), \ldots, (t'_m, c'_m)\}$. Then $(s, X) \xrightarrow{(a,v)} (s', X') \in \delta$ iff
  1. $s \xrightarrow{(a,v)} s'$ is a transition in $\hat{W}$, and
  2. $(t'_j, c'_j) \in X'$ if there exists $(t_i, c_i) \in X$, and a weight v' such that $t_i \xrightarrow{a,v'} t'_j$ and $c_i \xrightarrow{v,v'} c'_j$ are transitions in $\hat{W}$ and C, respectively.
- $(s, \{(t_1, c_1), \ldots, (t_n, c_n)\}) \in \mathcal{F}$ iff s and all t_i are accepting in $\hat{W}$, and all c_i is accepting in C.

Lemma 4. *Let W be a weighted automaton with regular safety comparator C for non-strict inequality. Then the size of* $\mathsf{Maximal}(W)$ *is* $|W| \cdot 2^{\mathcal{O}(|W| \cdot |C|)}$.

Proof (Proof sketch). A state $(s, \{(t_1, c_1), \ldots, (t_n, c_n)\})$ is non-accepting in the automata if one of s,t_i or c_j is non-accepting in underlying automata $\hat{W}$ and the comparator. Since $\hat{W}$ and the comparator automata are safety, all outgoing transitions from a non-accepting state go to non-accepting state in the underlying automata. Therefore, all outgoing transitions from a non-accepting state in $\mathsf{Maximal}(W)$ go to non-accepting state in $\mathsf{Maximal}(W)$. Therefore, $\mathsf{Maximal}(W)$ is a safety automaton. To see correctness of the transition relation, one must prove that transitions of type (1.) satisfy condition (a), while transitions of type (2.) satisfy condition (b). $\mathsf{Maximal}(W)$ forms the conjunction of (a) and (b), hence accepts the language of maximal words of W.

A similar construction proves that the maximal automata of weighted automata W with regular safety comparator C for strict inequality contains $|W| \cdot 2^{\mathcal{O}(|W| \cdot |C|)}$ states. In this case, however, the maximal automaton may not be a safety automaton. Therefore, Lemma 4 generalizes to:

Corollary 3. *Let W be a weighted automaton with regular safety/co-safety comparator C. Then* $\mathsf{Maximal}(W)$ *is a Büchi automaton of size* $|W| \cdot 2^{\mathcal{O}(|W| \cdot |C|)}$.

Counterexample Automaton. This section covers the construction of the counterexample automaton. Given weighted-automata P and Q, an annotated word (w, wt_P) in annotated automata $\hat{P}$ is a *counterexample word* of $P \subseteq Q$ (or $P \subset Q$) if there exists (w, wt_Q) in $\mathsf{Maximal}(Q)$ s.t. $wt(wt_P) > wt(wt_Q)$ (or $wt(wt_P) \geq wt(wt_Q)$). Clearly, annotated word (w, wt_P) is a counterexample word iff there exists a counterexample run of w with weight-sequence wt_P in P.

For this section, we abbreviate strict and non-strict to strct and nstrct, respectively. For $\mathsf{inc} \in \{\mathsf{strct}, \mathsf{nstrct}\}$, the *counterexample automaton* for inc-quantitative inclusion, denoted by $\mathsf{Counterexample}(\mathsf{inc})$, is the automaton that contains all counterexample words of the problem instance. We construct the counterexample automaton as follows:

Lemma 5. *Let P, Q be weighted-automata with regular safety/co-safety comparators. For $\mathsf{inc} \in \{\mathsf{strct}, \mathsf{nstrct}\}$, $\mathsf{Counterexample}(\mathsf{inc})$ is a Büchi automaton.*

Proof. We construct Büchi automaton $\mathsf{Counterexample}(\mathsf{inc})$ for $\mathsf{inc} \in \{\mathsf{strct}, \mathsf{nstrct}\}$ that contains the counterexample words of inc-quantitative inclusion. Since the comparator are regular safety/co-safety, $\mathsf{Maximal}(Q)$ is a Büchi automaton (Corollary 3). Construct the product $\hat{P} \times \mathsf{Maximal}(Q)$ such that transition $(p_1, q_1) \xrightarrow{a,v_1,v_2} (p_1, q_2)$ is in the product iff $p_1 \xrightarrow{a,v_1} p_1$ and $q_1 \xrightarrow{a,v_2} q_2$ are transitions in $\hat{P}$ and $\mathsf{Maximal}(Q)$, respectively. A state (p, q) is accepting if both p and q are accepting in $\hat{P}$ and $\mathsf{Maximal}(Q)$. One can show that the product accepts (w, wt_P, wt_Q) iff (w, wt_P) and (w, wt_Q) are words in $\hat{P}$ and $\mathsf{Maximal}(Q)$, respectively.

If $\mathsf{inc} = \mathsf{strct}$, intersect $\hat{P} \times \mathsf{Maximal}(Q)$ with comparator for $\geq$. If $\mathsf{inc} = \mathsf{nstrct}$, intersect $\hat{P} \times \mathsf{Maximal}(Q)$ with comparator for $>$. Since the comparator is a safety or co-safety automaton, the intersection is taken without the cyclic counter. Therefore, $(s_1, t_1) \xrightarrow{a,v_1,v_2} (s_2, t_2)$ is a transition in the intersection iff $s_1 \xrightarrow{a,v_1,v_2} s_2$ and $t_1 \xrightarrow{v_1,v_2} t_2$ are transitions in the product and the appropriate comparator, respectively. State (s, t) is accepting if both s and t are accepting. The intersection will accept (w, wt_P, wt_Q) iff (w, wt_P) is a counterexample of inc-quantitative inclusion. $\mathsf{Counterexample}(\mathsf{inc})$ is obtained by projecting out the intersection as follows: Transition $m \xrightarrow{a,v_1,v_2} n$ is transformed to $m \xrightarrow{a,v_1} n$. □

Quantitative Inclusion and DS-inclusion. In this section, we give the final algorithm for quantitative inclusion with regular safety/co-safety comparators. Since DS-comparators are regular safety/co-safety comparators, this gives us an algorithm for DS-inclusion with improved complexity than previous results.

Theorem 4. *Let P, Q be weighted-automata with regular safety/co-safety comparators. Let $C_{\leq}$ and $C_{<}$ be the comparators for $\leq$ and $<$, respectively. Then*

- *Strict quantitative inclusion $P \subset Q$ is reduced to emptiness checking of a Büchi automaton of size $|P||C_{\leq}||Q| \cdot 2^{\mathcal{O}(|Q| \cdot |C_{<}|)}$.*
- *Non-strict quantitative inclusion $P \subseteq Q$ is reduced to emptiness checking of a Büchi automaton of size $|P||C_{<}||Q| \cdot 2^{\mathcal{O}(|Q| \cdot |C_{<}|)}$.*

Proof. Strict and non-strict are abbreviated to strct and nstrct, respectively. For inc $\in$ {strct, nstrct}, inc-quantitative inclusion holds iff Counterexample(inc) is empty. Size of Counterexample(inc) is the product of size of P, Maximal(Q) (Corollary 3), and the appropriate comparator as described in Lemma 5. □

In contrast, quantitative inclusion with regular comparators reduces to emptiness of a Büchi automaton with $|P| \cdot 2^{\mathcal{O}(|P||Q||C| \cdot \log(|P||Q||C|))}$ states [12]. The $2^{\mathcal{O}(n \log n)}$ blow-up is unavoidable due to Büchi complementation. Hence, quantitative inclusion with regular safety/co-safety has lower worst-case complexity.

Lastly, we use the results of developed in previous sections to solve DS-inclusion. Since DS-comparators are regular safety/co-safety (Corollary 1), an immediate consequence of Theorem 4 is an improvement in the worst-case complexity of DS-inclusion in comparison to prior results with regular DS-comparators. Furthermore, since the regular safety/co-safety DS-comparators are of the same size for all inequalities (Theorem 3), we get:

Corollary 4. *Let P, Q be weighted-automata, and C be a regular safety/co-safety DS-comparator with integer discount-factor $d > 1$.* Strict DS-inclusion *reduces to emptiness checking of a* safety automaton *of size $|P||C||Q| \cdot 2^{\mathcal{O}(|Q| \cdot |C|)}$.*

Proof (Proof sketch). When comparator for non-strict inequality is safety-automaton, as it is for DS-comparator, the maximal automaton is a safety automaton (Lemma 3). One can then show that the counterexample automata is also a safety automaton.

A similar argument proves *non-strict DS-inclusion* reduces to emptiness of a *weak-Büchi automaton* [27] of size $|P||C||Q| \cdot 2^{\mathcal{O}(|Q| \cdot |C|)}$ (see Appendix).

Corollary 5 ([DS-inclusion with safety/co-safety comparator**).** *Let P, Q be weighted-automata, and C be a regular (co)-safety DS-comparator with integer discount-factor $d > 1$.The complexity of DS-inclusion is $|P||C||Q| \cdot 2^{\mathcal{O}(|Q| \cdot |C|)}$.*

4 Implementation and Experimental Evaluation

The goal of the empirical analysis is to examine performance of DS-inclusion with integer discount-factor with safety/co-safety comparators against existing tools to investigate the practical merit of our algorithm. We compare against (a) Regular-comparator based tool QuIP, and (b) DS-determinization and linear-programming tool DetLP.

QuIP is written in C++, and invokes state-of-the-art Büchi language inclusion-solver RABIT [2]. We enable the `-fast` flag in RABIT, and tune its Java-threads with Xss, Xms, Xmx set to 1GB, 1GB and 8GB, respectively. DetLP is also written in C++, and uses linear programming solver GLPSOL provided by GLPK (GNU Linear Prog. Kit) [1]. We compare these tools along two axes: runtime and number of benchmarks solved.

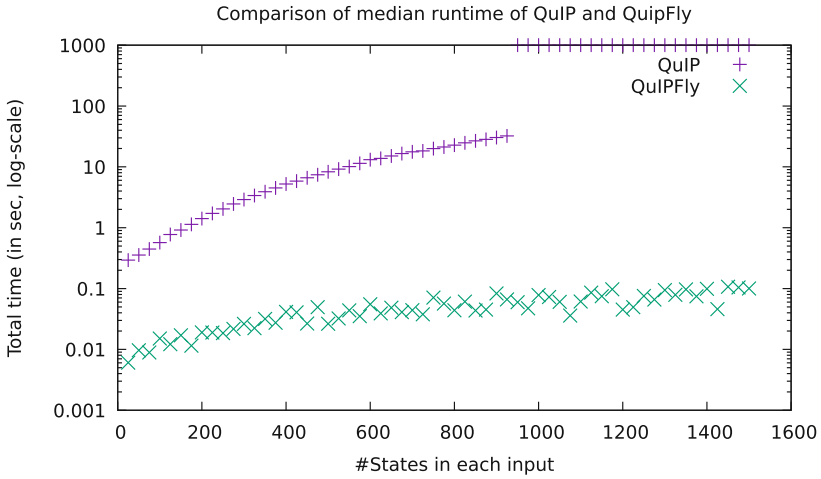

Fig. 1. $s_P = s_Q$ on x-axis, $wt = 4$, $\delta = 3$, $d = 3$, $P \subset Q$

Implementation Details. The algorithm for strict-DS-inclusion with integer discount factor $d > 1$ proposed in Corollary 4 and non-strict DS-inclusion checks for emptiness of the counterexample automata. A naive algorithm will construct the counterexample automata fully, and then check if they are empty by ensuring the absence of an *accepting lasso*.

We implement a more efficient algorithm. In our implementation, we make use of the fact that the constructions for DS-inclusion use subset-construction intermediate steps. This facilitates an *on-the-fly procedure* since successor states of state in the counterexample automata can be determined directly from input weighted automata and the comparator automata. The algorithm terminates as soon as an accepting lasso is detected. When an accepting lasso is absent, the algorithm traverses all states and edges of the counterexample automata.

We implement the optimized on-the-fly algorithm in a prototype QuIPFly. QuIPFly is written in Python 2.7.12. QuIPFly employs basic implementation-level optimizations to avoid excessive re-computation.

Design and Setup for Experiments. Due to lack of standardized benchmarks for weighted automata, we follow a standard approach to performance evaluation of automata-theoretic tools [3,30,38] by experimenting with *randomly generated* benchmarks, using random benchmark generation procedure described in [11].

The parameters for each experiment are number of states s_P and s_Q of weighted automata, transition density δ, maximum weight wt, integer discount-factor d, and $\mathsf{inc} \in \{\mathsf{strct}, \mathsf{nstrct}\}$. In each experiment, weighted automata P and Q are randomly generated, and runtime of inc-DS-inclusion for all three tools is reported with a timeout of 900 s. We run the experiment for each parameter tuple 50 times. All experiments are run on a single node of a high-performance cluster consisting of two quad-core Intel-Xeon processor running at 2.83 GHz,

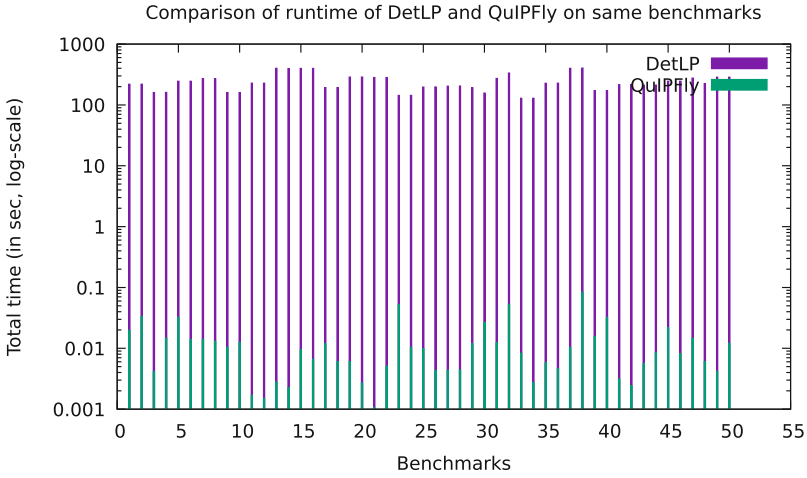

Fig. 2. $s_P = s_Q = 75$, $wt = 4$, $\delta = 3$, $d = 3$, $P \subset Q$

with 8 GB of memory per node. We experiment with $s_P = s_Q$ ranging from 0–1500 in increments of 25, $\delta \in \{3, 3.5, 4\}$, $d = 3$, and $wt \in \{d^1 + 1, d^3 - 1, d^4 - 1\}$.

Observations and Inferences.[1] For clarity of exposition, we present the observations for only one parameter-tuple. Trends and observations for other parameters were similar.

QuIPFly Outperforms. QuIP by at least an order of magnitude in runtime. Figure 1 plots the median runtime of all 50 experiments for the given parameter-values for QuIP and QuIPFly. More importantly, QuIPFly solves all of our benchmarks within a fraction of the timeout, whereas QuIP struggled to solve at least 50% of the benchmarks with larger inputs (beyond $s_P = s_Q = 1000$). Primary cause of failure is memory overflow inside RABIT. We conclude that regular safety/co-safety comparators outperform their regular counterpart, giving credit to the simpler subset-constructions vs. Büchi complementation.

QuIPFly Outperforms. DetLP comprehensively in runtime and in number of benchmarks solved. We were unable to plot DetLP in Fig. 1 since it solved fewer than 50% benchmarks even with small input instances. Figure 2 compares the runtime of both tools on the same set of 50 benchmarks for a representative parameter-tuple on which all 50 benchmarks were solved. The plot shows that QuIPFly beats DetLP by 2–4 orders of magnitude on all benchmarks.

Overall Verdict. Overall, QuIPFly outperforms QuIP and DetLP by a significant margin along both axes, runtime and number of benchmarks solved. This analysis gives unanimous evidence in favor of our safety/co-safety approach to solving DS-inclusion.

[1] Figures are best viewed online and in color.

5 Concluding Remarks

The goal of this paper was to build scalable algorithms for DS-inclusion. To this end, this paper furthers the understanding of language-theoretic properties of discounted-sum aggregate function by demonstrating that DS-comparison languages form safety and co-safety languages, and utilizes these properties to obtain a decision procedure for DS-inclusion that offers both tighter theoretical complexity and improved scalability. All in all, the key insights of this work are:

1. Pure automata-theoretic techniques of DS-comparator are better for DS-inclusion;
2. In-depth language-theoretic analysis improve both theoretical complexity and practical scalability of DS-inclusion;
3. DS-comparators are compact deterministic safety or co-safety automata.

To the best of our knowledge, this is the first work that applies language-theoretic properties such as safety/co-safety in the context of quantitative reasoning.

More broadly, this paper demonstrates that the close integration of language-theoretic and quantitative properties can render novel algorithms for quantitative reasoning that can benefit from advances in qualitative reasoning.

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Clock Bound Repair for Timed Systems

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Abstract. We present algorithms and techniques for the repair of timed system models, given as networks of timed automata (NTA). The repair is based on an analysis of timed diagnostic traces (TDTs) that are computed by real-time model checking tools, such as UPPAAL, when they detect the violation of a timed safety property. We present an encoding of TDTs in linear real arithmetic and use the MaxSMT capabilities of the SMT solver Z3 to compute possible repairs to clock bound values that minimize the necessary changes to the automaton. We then present an admissibility criterion, called functional equivalence, that assesses whether a proposed repair is admissible in the overall context of the NTA. We have implemented a proof-of-concept tool called TARTAR for the repair and admissibility analysis. To illustrate the method, we have considered a number of case studies taken from the literature and automatically injected changes to clock bounds to generate faulty mutations. Our technique is able to compute a feasible repair for 91% of the faults detected by UPPAAL in the generated mutants.

Keywords: Timed automata · Automated repair · Admissibility of repair · TARTAR tool

1 Introduction

The analysis of system design models using model checking technology is an important step in the system design process. It enables the automated verification of system properties against given design models. The automated nature of model checking facilitates the integration of the verification step into the design process since it requires no further intervention of the designer once the model has been formulated and the property has been specified.

Often it is sufficient to abstract from real time aspects when checking system properties, in particular when the focus is on functional aspects of the system. However, when non-functional properties, such as response times or the timing of periodic behavior, play an important role, it is necessary to incorporate real time aspects into the models and the specification, as well as to use specialized real-time model checking tools, such as UPPAAL [6], Kronos [31] or opaal [11] during the verification step.

Next to the automatic nature of model checking, the ability to return counterexamples, in real-time model checking often referred to as timed diagnostic traces (TDT), is

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a further practical benefit of the use of model checking technology. A TDT describes a timed sequence of steps that lead the design model from the initial state of the system into a state violating a real-time property. A TDT neither constitutes a causal explanation of the property violation, nor does it provide hints as to how to correct the model.

In this paper we describe an automated method that computes proposals for possible repairs of a network of timed automata (NTA) that avoid the violation of a timed safety property. Consider the TDT depicted as a time annotated sequence diagram [5] in Fig. 1. This scenario describes a simple message exchange where the process `dbServer` sends a message `req` to process `db` which, after some processing steps returns a message `ser` to `dbServer`. Assume a requirement on the system to be that the time from sending `req` to receiving `ser` is not to be more than 4 time units. Assume that the timing interval annotations on the sequence diagram represent the minimum and maximum time for the message transmission and processing steps that the NTA, from which the diagram has been derived, permits. It is then easy to see that it is possible to execute the system in such a way that this property is violated.

Various changes to the underlying NTA model, depicted in Fig. 2, may avoid this property violation. For instance, the maximum time it takes to transmit the `req` and `ser` messages can be constrained to be at most 1 time unit, respectively. Alternatively, it may be possible to avoid the property violation by reducing two of the three timings by 0.5 time units. In any case, proposing such changes to the model may either serve to correct clerical mistakes made during the editing of the model, or point to necessary changes in the dimensioning of its time resources, thus contributing to improved design space exploration.

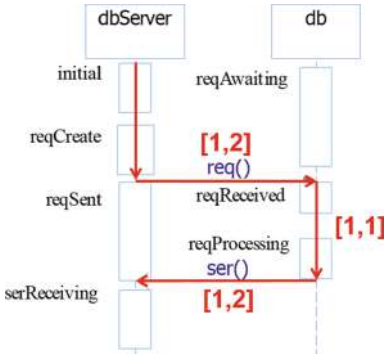


Fig. 1. TDT represented as a sequence diagram with timing annotations

The repair method described in this paper relies on an encoding of a TDT as a constraint system in linear real arithmetic. This encoding provides a symbolic abstract semantics for the TDT by constraining the sojourn time of the NTA in the locations visited along the trace. The constraint system is then augmented by auxiliary model variation variables which represent syntactic changes to the NTA model, for instance the variation of a location invariant condition or a transition guard. We assert that the thus modified constraint system implies the non-reachability of a violation. At the same time, we assert that the model variation variables have a value that implies that no change of the NTA model will occur, for instance by setting a clock bound variation variable to 0. This renders the resulting constraint system unsatisfiable.

In order to compute a repair, we derive a partial MaxSMT instance by turning the constraints that disable any repair into soft constraints. We solve this MaxSMT instance using the SMT solver Z3 [25]. If the MaxSMT instance admits a solution, the resulting model provides values of the model variation variables. These values indicate a repair

of the NTA model which entails that along the sequence of locations represented by the TDT, the property violation will no longer be reachable.

In a next step it is necessary to check whether the computed repair is an admissible repair in the context of the full NTA. This is important since the repair was computed locally with respect to only a single given TDT. Thus, it is necessary to define a notion of admissibility that is reasonable and helpful in this setting. To this end, we propose the notion of *functional equivalence* which states that as a result of the computed repair, neither erstwhile existing functional behavior will be purged, nor will new functional behavior be added. Functional behavior in this sense is represented by languages accepted by the untimed automata of the unrepaired and the repaired NTAs. Functional equivalence is then defined as equivalence of the languages accepted by these automata. We propose a zone-based automaton construction for implementing the functional equivalence test that is efficient in practice.

We have implemented our proposed method in a proof-of-concept tool called TarTar[1]. Our evaluation of TarTar is based on several non-trivial NTA models taken from the literature, including the frequently considered Pacemaker model [19]. For each model, we automatically generate mutants by injecting clock bound variations which we then model check using UPPAAL and repair using TarTar. The evaluation shows that our technique is able to compute an admissible repair for 91% of the detected faults.

Related Work. There are relatively few results available on a formal treatment of TDTs. The zone based approach to real-time model checking, which relies on a constraint-based abstraction of the state space, is proposed in [14]. The use of constraint solving to perform reachability analysis for NTAs is described in [30]. This approach ultimately leads to the on-the-fly reachability analysis algorithm used in UPPAAL [7]. [12] defines the notion of a time-concrete UPPAAL counterexample. Work documented in [27] describes the computation of concrete delays for symbolic TDTs. The above cited approaches address neither fault analysis nor repair for TDTs. Our use of MaxSMT solvers for computing minimal repairs is inspired by the use MaxSAT solvers for fault localization in C programs, which was first explored in the BugAssist tool [20,21]. Our approach also shares some similarities with syntax-guided synthesis [2,28], which has also been deployed in the context of program repair [22]. One key difference is how we determine the admissibility of a repair in the overall system, which takes advantage of the semantic restrictions imposed by timed automata.

Structure of the Paper. We will introduce the automata and real-time concepts needed in our analysis in Sect. 2. In Sect. 3 we present the logical formalization of TDTs. The repair and admissibility analyses are presented in Sects. 4 and 5, respectively. We report on tool development, experimental evaluation and case studies in Sects. 6 and 7 concludes.

[1] TarTar and links to all models used in this paper can be found at URL https://github.com/sen-uni-kn/tartar.

2 Preliminaries

The timed automaton model that we use in this paper is adapted from [7]. Given a set of *clocks* C, we denote by $\mathcal{B}(C)$ the set of all *clock constraints* over C, which are conjunctions of *atomic clock constraints* of the form $c \sim n$, where $c \in C$, $\sim \in \{<, \leq, =, \geq, >\}$ and $n \in \mathbb{N}$. A *timed automaton (TA)* T is a tuple $T = (L, l^0, C, \Sigma, \Theta, I)$ where L is a finite set of locations, $l^0 \in L$ is an initial location, C is a finite set of clocks, Σ is a set of action labels, $\Theta \subseteq_{fin} L \times \mathcal{B}(C) \times \Sigma \times 2^C \times L$ is a set of *actions*, and $I : L \to \mathcal{B}(C)$ denotes a labeling of locations with clock constraints, referred to as location invariants. For $\theta \in \Theta$ with $\theta = (l, g, a, r, l')$ we refer to g as the *guard* of θ and to r as its *clock resets*.

The operational semantics of T is given by a timed transition system consisting of states $s = (l, u)$ where l is a location and $u : C \to \mathbb{R}_+$ is a *clock valuation*. The initial state s_0 is (ℓ, u_0) where u_0 maps all clocks to 0. For a clock constraint B we write $u \models B$ iff B evaluates to true in u. There are two types of transitions. An *action transition* models the execution of an action whose guard is satisfied. These transitions are instantaneous and reset the specified clocks. The passing of time in a location is modeled by *delay transitions*. Both types of transitions guarantee that location invariants are satisfied in the pre and post state. Formally, we have $(l, u) \xrightarrow{t} (l', u')$ iff

- (action transition) $t = (l, g, a, r, l') \in \Theta$, $u \models I(l) \wedge g$, $u' \models I(l')$ and for all clocks $c \in C$, $u'(c) = 0$ if $c \in r$ and $u'(c) = u(c)$ otherwise; or
- (delay transition) $t \in \mathbb{R}_+$, $u \models I(l)$, $u' \models I(l)$ and $u' = u + t$.

Definition 1. *A* symbolic timed trace *(STT) of T is a sequence of actions $S = \theta_0, \ldots, \theta_{n-1}$. A* realization *of S is a sequence of delay values $\delta_0, \ldots, \delta_n$ such that there exists states $s_0, \ldots, s_n, s_{n+1}$ with $s_i \xrightarrow{\delta_i} \xrightarrow{\theta_i} s_{i+1}$ for all $i \in [0, n)$ and $s_n \xrightarrow{\delta_n} s_{n+1}$. We say that a STT is* feasible *if it has at least one realization.*

Property Specification. We focus on the analysis of timed safety properties, which we characterize by an invariant formula that has to hold for all reachable states of a TA. These properties state, for instance, that there are certain locations in which the value of a clock variable is not above, equal to or below a certain (integer) bound. Formally, let $T = (L, l^0, C, \Sigma, \Theta, I)$ be a TA. A *timed safety property* Π is a Boolean combination of atomic clock constraints and *location predicates* $@l$ where $l \in L$. A location predicate $@l$ holds in a state (l', u) of T iff $l' = l$. We say that a STT S witnesses a violation of Π in T if there exists a realization of S whose induced final state does not satisfy Π. We refer to such an STT as a *timed diagnostic trace* of T for Π.

T satisfies Π iff all its reachable states satisfy Π. This problem can be decided using model checking tools such as Kronos [31] and UPPAAL [6]. UPPAAL in particular computes a finite abstraction of the state space of an NTA using a zone graph construction. Reachability analysis is then performed by an on-the-fly search of the zone graph. If the property is violated, the tool generates a feasible TDT that witnesses the violation. The objective of our work is to analyze TDTs and to propose repairs for the property violation that they represent. We use TDTs generated by the UPPAAL tool in our implementation, but we maintain that our results can be adapted to any other tool producing TDTs.

We further note that UPPAAL takes a *network of timed automata* (NTA) as input, which is a CCS [24] style parallel composition of timed automata $T_1 \mid \ldots \mid T_n$. Since our analysis and repair techniques focus on timing-related errors rather than synchronization errors, we use TAs rather than NTAs in our formalization. However, our implementation works on NTAs.

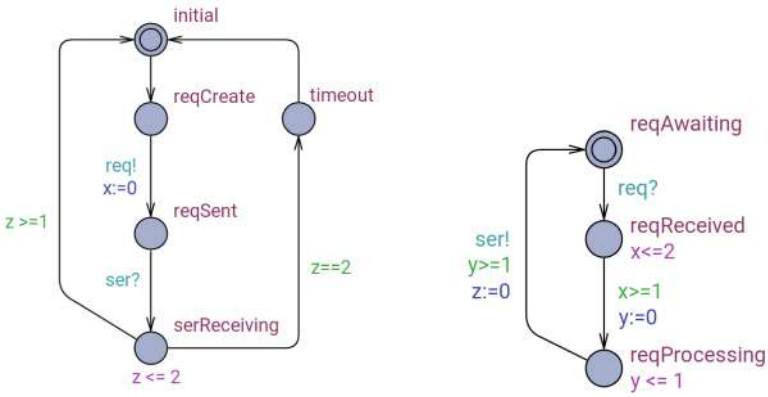
Example 1. The running example that we use throughout the paper consists of an NTA of two timed automata, depicted in Fig. 2. As alluded to in the introduction, the TAs `dbServer` and `db` synchronize via the exchange of messages modeled by the pairs of send and receive actions `req!` and `req?`, respectively, `ser!` and `ser?`. The transmission time of the `req` message is controlled by the clock variable `x` and can range between 1 and 2 time units. This is achieved by the location invariant `x<=2` on the `reqReceived` location in `db` together with the transition guard `x>=1` on the transition from `reqReceived` to `reqProcessing`. A similar mechanism using clock variable `z` is used to constrain the timing of the transfer of message `ser` to be within 1 and 2 time units. The processing time in `dbServer` is constrained to exactly 1 time unit by the location invariant `y<=1` and the transition guard `y>=1`. In `dbServer`, a transition to location `timeout` can be triggered when the guard `z==2` is satisfied in location `serReceiving`. The clock variable `x`, which is not reset until the next `req` message is sent, is recording the time that has elapsed since sending `req` and is used in location `serReceiving` in order to verify if more than 4 time units have passed since `req` was sent. The timed safety property that we will consider for our example is $\Pi = \neg@\texttt{dbServer.serReceiving} \vee (x < 4)$. For the violation of this property, UPPAAL produces the TDT $S = \theta_0 \ldots \theta_3$ where

$$\theta_0 = ((\texttt{initial}, \texttt{reqAwaiting}), \emptyset, \tau, \emptyset, (\texttt{reqCreate}, \texttt{reqAwaiting}))$$
$$\theta_1 = ((\texttt{reqCreate}, \texttt{reqAwaiting}), \emptyset, \tau, \{x\}, (\texttt{reqSent}, \texttt{reqReceived}))$$
$$\theta_2 = ((\texttt{reqSent}, \texttt{reqReceived}), \{x \geq 1\}, \tau, \{y\}, (\texttt{reqSent}, \texttt{reqProc.}))$$
$$\theta_3 = ((\texttt{reqSent}, \texttt{reqProc.}), \{y \geq 1\}, \tau, \{z\}, (\texttt{serReceiving}, \texttt{reqAwait.})).$$

3 Logical Encoding of Timed Diagnostic Traces

Our analysis relies on a logical encoding of TDTs in the theory of quantifier-free linear real arithmetic. For the remainder of this paper, we fix a TA $T = (L, l^0, C, \Sigma, \Theta, I)$ with a safety property Π and assume that $S = \theta_0, \ldots, \theta_{n-1}$ is an STT of T. We use the following notation for our logical encoding where $j \in [0, n+1]$ is a position in a realization of S and $c \in C$ is a clock:

- l_j denotes the location of the pre state of θ_j for $j < n$ and the location of the post state of θ_{j-1} for $j = n$.
- c_j denotes the value of clock variable c when reaching the state at position j.
- δ_j denotes the delay of the delay transition leaving the state at position $j \leq n$.
- reset_j denotes the set of clock variables that are being reset by action θ_j for $j < n$.
- $\mathit{ibounds}(c, l)$ denotes the set of pairs $(\beta, \sim)$ such that the atomic clock constraint $c \sim \beta$ appears in the location invariant $I(l)$.



(a) Timed Automaton `dbServer` (b) Timed Automaton `db`

Fig. 2. Network of timed automata - running example

– $gbounds(c, \theta)$ denotes the set of pairs $(\beta, \sim)$ such that the atomic clock constraint $c \sim \beta$ appears in the guard of action θ.

To illustrate the use of *ibounds*, assume location l to be labeled with invariants $x > 2 \wedge x \leq 4 \wedge y \leq 1$, then $ibounds(x, l) = \{(2, >), (4, \leq)\}$. The usage of *gbounds* is accordingly.

Definition 2. *The* timed diagnostic trace constraint system *associated with STT S is the conjunction $\mathcal{T}$ of the following constraints:*

$$\mathcal{C}_0 \equiv \bigwedge_{c \in C} c_0 = 0 \qquad \textit{(clock initialization)}$$

$$\mathcal{A} \equiv \bigwedge_{j \in [0,n]} \delta_j \geq 0 \qquad \textit{(time advancement)}$$

$$\mathcal{R} \equiv \bigwedge_{c \in reset_j,} c_{j+1} = 0 \qquad \textit{(clock resets)}$$

$$\mathcal{D} \equiv \bigwedge_{c \notin reset_j} c_{j+1} = c_j + \delta_j \qquad \textit{(sojourn time)}$$

$$\mathcal{I} \equiv \bigwedge_{(\beta,\sim) \in ibounds(c,l_j)} c_j \sim \beta \wedge c_j + \delta_j \sim \beta \qquad \textit{(location invariants)}$$

$$\mathcal{G} \equiv \bigwedge_{(\beta,\sim) \in gbounds(c,\theta_j)} c_j + \delta_j \sim \beta \qquad \textit{(transition guards)}$$

$$\mathcal{L} \equiv @l_n \wedge \bigwedge_{l \neq l_n} \neg @l \qquad \textit{(location predicates)}$$

Let further $\Phi \equiv \Pi[\mathbf{c}_{n+1}/\mathbf{c}]$ where $\Pi[\mathbf{c}_{n+1}/\mathbf{c}]$ is obtained from Π by substituting all occurrences of clocks $c \in C$ with c_{n+1}. Then the Π-extended TDT constraint system associated with S is defined as $\mathcal{T}^{\Pi} = \mathcal{T} \wedge \neg\Phi$.

To illustrate the encoding consider the transition Θ_3 of the TDT in Example 1 corresponding to the transition from state (`reqSent`, `reqProcessing`) to state (`serReceiving`, `reqAwaiting`) while resetting clock `z` in the NTA of Fig. 2. The encoding for the constraints on the clocks `x`, `y` and `z` is as following: $y_3 + d_3 \geq 1$, $z_4 = 0$, $x_4 = x_3 + d_3$ and $y_4 = y_3 + d_3$.

Lemma 1. *$\delta_0^c, \ldots, \delta_n^c$ is a realization of an STT S iff there exists a satisfying variable assignment ι for $\mathcal{T}$ such that for all $j \in [0, n]$, $\iota(\delta_j) = \delta_j^c$.*

Theorem 1. *An STT S witnesses a violation of Π in T iff $\mathcal{T}^{\Pi}$ is satisfiable.*

4 Repair

We propose a repair technique that analyzes the responsibility of clock bound values occurring in a single TDT for causing the violation of a specification Π. The analysis suggests possible syntactic repairs. In a second step we define an admissibility test that assesses the admissibility of the repair in the context of the complete TA model. Throughout this section, we assume that S is a TDT for T and Π.

Clock Bound Variation. We introduce *bound variation variables* v that stand for *correction values* that the repair will add to the clock bounds occurring in location invariants and transition guards. The values are chosen such that none of the realizations of S in the modified automaton still witnesses a violation of Π. This is done by defining a new constraint system that captures the conditions on the variable v under which the violation of Π will not occur in the corresponding trace of the modified automaton. Using this constraint system, we then define a maximum satisfiability problem whose solution minimizes the number of changes to T that are needed to achieve the repair.

Recall that the clock bounds occurring in location invariants and in transition guards are represented by the *ibounds* and *gbounds* sets defined for the TDT S. Notice that each clock variable c may be associated with $m_{c,l}$ different clock bounds in the location invariant of l, denoted by the set $\mathit{ibounds}(c, l) = \{(\beta_1^{c,l}, \sim_1^{c,l}), \ldots, (\beta_{m_{c,l}}^{c,l}, \sim_{m_{c,l}}^{c,l})\}$. Similarly, we enumerate the bounds in $\mathit{gbounds}(c, \theta)$ as $(\beta_k^{c,\theta}, \sim_k^{c,\theta})$. To reduce notational clutter, we let the meta variable r stand for the pairs of the form c, l or c, θ. We then introduce bound variation variables v_k^r describing the possible static variation in the TA code for the clock bound β_k^r and modify the TDT constraint system accordingly. A variation of the bounds only affects the location invariant constraints $\mathcal{I}$ and the transition guard constraints $\mathcal{G}$. We thus define an appropriate invariant variation constraint $\mathcal{I}^{bv}$ and guard variation constraint $\mathcal{G}^{bv}$ that capture the clock bound modifications:

$$\mathcal{I}^{bv} \equiv \bigwedge_{(\beta_k^r, \sim_k^r) \in \mathit{ibounds}(c, l_j)} c_j \sim_k^r (\beta_k^r + v_k^r) \wedge c_j + \delta_j \sim_k^r (\beta_k^r + v_k^r)$$

$$\mathcal{G}^{bv} \equiv \bigwedge_{(\beta_k^r, \sim_k^r) \in \mathit{gbounds}(c, \theta_j)} c_j + \delta_j \sim_k^r (\beta_k^r + v_k^r)$$

We also need constraints ensuring that the modified clock bounds remain positive:

$$\mathcal{Z}^{bv} \equiv \bigwedge_{(\beta_k^r, \sim_k^r) \in \mathit{ibounds}(c,l_j) \cup \mathit{gbounds}(c,\theta_j)} \beta_k^r + v_k^r \geq 0$$

Putting all of this together we obtain the *bound variation TDT constraint system*

$$\mathcal{T}^{bv} \equiv \mathcal{C}_0 \wedge \mathcal{A} \wedge \mathcal{R} \wedge \mathcal{D} \wedge \mathcal{I}^{bv} \wedge \mathcal{G}^{bv} \wedge \mathcal{Z}^{bv} \wedge \mathcal{L}$$

which captures all realizations of S in TAs T^{bv} that are obtained from T by modifying the clock bounds β_k^r by some semantically consistent variations v_k^r.

Consider the bound variation for the guard $y \geq 1$ of transition Θ_3 in Example 1. The modified guard constraint, a conjunct in $\mathcal{G}^{bv}$, is $y_3 + d_3 \geq 1 + v_3^y$. The corresponding non-negativity constraint from $\mathcal{Z}^{bv}$ is $1 + v_3^y \geq 0$.

Repair by Bound Variation Analysis. The objective of the bound variation analysis is to provide hints to the system designer regarding which minimal syntactic changes to the considered model might prevent the violation of property Π. Minimality here is considered with respect to the number of clock bound values in invariants and guards that need to be changed.

We implement this analysis by using the bound variation TDT constraint system $\mathcal{T}^{bv}$ to derive an instance of the partial MaxSMT problem whose solutions yield candidate repairs for the timed automaton T. The partial MaxSMT problem takes as input a finite set of assertion formulas belonging to a fixed first-order theory. These assertions are partitioned into *hard* and *soft* assertions. The hard assertions $\mathcal{F}_H$ are assumed to hold and the goal is to find a maximizing subset $\mathcal{F}' \subseteq \mathcal{F}_S$ of the soft assertions such that $\mathcal{F}' \cup \mathcal{F}_H$ is satisfiable in the given theory.

For our analysis, the hard assertions consist of the conjunction

$$\mathcal{F}_H^{bv} \equiv (\exists \delta_j, c_j . \mathcal{T}^{bv}) \wedge (\forall \delta_j, c_j . \mathcal{T}^{bv} \Rightarrow \Phi).$$

Note that the free variables of $\mathcal{F}_H^{bv}$ are exactly the bound variation variables v_k^r. Given a satisfying assignment ι for $\mathcal{F}_H^{bv}$, let T_ι be the timed automaton obtained from T by adding to each clock bound β_k^r the according variation value $\iota(v_k^r)$ and let S_ι be the TDT corresponding to S in T_ι. Then $\mathcal{F}_H^{bv}$ guarantees that

1. S_ι is feasible, and
2. S_ι has no realization that witnesses a violation of Π in T_ι.

We refer to such an assignment ι as a *local clock bound repair* for T and S. To obtain a minimal local clock bound repair, we use the soft assertions given by the conjunction

$$\mathcal{F}_S^{bv} \equiv \bigwedge_{(\beta_k^r, \_) \in \mathit{ibounds}(c,l_j) \cup \mathit{gbounds}(c,\theta_j)} v_k^r = 0.$$

Clearly $\mathcal{F}_H^{bv} \wedge \mathcal{F}_S^{bv}$ is unsatisfiable because $\mathcal{T}^{bv} \wedge \mathcal{F}_S^{bv}$ is equisatisfiable with $\mathcal{T}$, and $\mathcal{T} \wedge \neg\Phi$ is satisfiable by assumption. However, if there exists at least one local clock

bound repair for T and S, then $\mathcal{F}_H^{bv}$ alone is satisfiable. In this case, the MaxSMT instance $\mathcal{F}_H^{bv} \cup \mathcal{F}_S^{bv}$ has at least one solution. Every satisfying assignment of such a solution corresponds to a local repair that minimizes the number of clock bounds that need to be changed in T.

Note that hard and soft assertions remain within a decidable logic. Using an SMT solver such as Z3, we can enumerate all the optimal solutions for the partial MaxSMT instance and obtain a minimal local clock bound repair from each of them.

Example 2. We have applied the bound variation repair analysis to the TDT from Example 1, using TarTar, which calls Z3. The following repairs were computed:

1. $v_1^{z,l_5} = -1$. This corresponds to a variation of the location invariant regarding clock `z` in location 5 of the TDT, corresponding to location `dbServer.serReceiving`, to read $z \leq 1$ instead of $z \leq 2$. This indicates that the violation of the bound on the total duration of the transaction, as indicated by a return to the `serReceiving` location and a value greater than 4 for clock `x`, can be avoided by ensuring that the time taken for transmitting the `ser` message to the `dbServer` is constrained to take exactly 1 time unit.
2. A further computed repair is $v_1^{x,l_2} = -1$. Interpreting this variation in the context of Example 1 means that location `db.reqReceived` will be left when the clock `x` has value 1. In other words, the transmission of the message `req` to the `db` takes exactly one time unit, not between 1 and 2 time units as in the unrepaired model.
3. Another possible repair implies the modification of two clock bounds. This is no longer an optimal solution and no further optimal solution exists. Notice that even non-optimal solutions might provide helpful insight for the designer, for instance if optimal repairs turn out not to be implementable, inadmissible or leading to a property violation. It is therefore meaningful to allow a practical tool implementation to compute more than just the optimal repairs.

5 Admissibility of Repair

The synthesized repairs that lead to a TA T_ι change the original TA T in fundamental ways, both syntactically and semantically. This brings up the question whether the synthesized repairs are admissible. In fact, one of the key questions is what notion of admissibility is meaningful in this context.

A *timed trace* [7] is a sequence of timed actions $\xi = (t_1, a_1), (t_2, a_2), \ldots$ that is generated by a run of a TA, where $t_i \leq t_{i+1}$ for all $i \geq 1$. The timed language for a TA T is the set of all its timed traces, which we denote by $\mathcal{L}_T(T)$. The untimed language of T consists of words over T's alphabet Σ so that there exists at least one timed trace of T forming this word. Formally, for a timed trace $\xi = (t_1, a_1), (t_2, a_2) \ldots$, the untime operator $\mu(\xi)$ returns an untimed trace $\xi_\mu = a_1 a_2 \ldots$. We define the untimed language $\mathcal{L}_\mu(T)$ of the TA T as $\mathcal{L}_\mu(T) = \{\mu(\xi) \mid \xi \in \mathcal{L}_T(T)\}$.

Let B be a Büchi automaton (BA) [10] over some alphabet Σ. We write $\mathcal{L}(B) \subseteq \Sigma^\omega$ for the language accepted by B. Similarly, we denote by $\mathcal{L}_f(B) \subseteq \Sigma^*$ the language accepted by B if it is interpreted as a nondeterministic finite automaton (NFA). Further, we write *pref*$(\mathcal{L}(B))$ to denote the set of all finite prefixes of words in $\mathcal{L}(B)$.

For a given NFA or BA M, the *closure* $\texttt{cl}(M)$ denotes the automaton obtained from M by turning all of its states into accepting states. We call M closed iff $M = \texttt{cl}(M)$. Notice that a Büchi automaton accepts a safety language if and only if it is closed [1].

Admissibility Criteria. From a *syntactic* point of view the repair obtained from a satisfying assignment ι of the MaxSMT instance ensures that T_ι is a syntactically valid TA model by, for instance, placing non-negativity constraints on repaired clock bounds. In case repairs alter right hand sides of clock constraints to rational numbers, this can easily be fixed by normalizing all clock constraints in the TA.

From a *semantic* perspective, the impact of the repairs is more profound. Since the repairs affect time bounds in location invariants and transition guards, as well as clock resets, the behavior of T_ι may be fundamentally different from the behavior of T.

- First, the computed repair for one property Π may render another property Π' violated. To check admissibility of the synthesized repair with respect to the set of all properties $\widehat{\Pi}$ in the system specification, a full re-checking of $\widehat{\Pi}$ is necessary.
- Second, a repair may have introduced zenoness and timelock [4] into T_ι. As discussed in [4], there exists both an over-approximating static test for zenoness as well as a model checking based precise test for timelocks that can be used to verify whether the repair is admissible in this regard.
- Third, due to changes in the possible assignment of time values to clocks, reachable locations in the TA T may become unreachable in T_ι, and vice versa. On the one hand, this means that some functionalities of the system may no longer be provided since part of the actions in T will no longer be executable in T_ι, and vice versa. Further, a reduction in the set of reachable locations in T_ι compared to T may mean that certain locations with property violations in T are no longer reachable in T_ι, which implies that certain property violations are masked by a repair instead of being fixed. On the other hand, the repair leading to locations becoming reachable in T_ι that were unreachable in T may have the effect that previously unobserved property violations become visible and that T_ι possesses functionality that T does not have, which may or may not be desirable.

It should be pointed out that we assess admissibility of a repair leading to T_ι with respect to a given TA model T, and not with respect to a correct TA model T^* satisfying Π.

Functional Equivalence. While various variants of semantic admissibility may be considered, we are focusing on a notion of admissibility that ensures that a repair does not unduly change the functional behavior of the modeled system while adhering to the timing constraints of the repaired system. We refer to this as *functional equivalence*. The functional capabilities of a timed system manifest themselves in the sets of action or transition traces that the system can execute. For TAs T and T_ι this means that we need to consider the languages over the action or transition alphabets that these TAs define. Considering the timed languages of T and T_ι, we can state that $\mathcal{L}_T(T) \neq \mathcal{L}_T(T_\iota)$ since the repair forces at least one timed trace to be purged from $\mathcal{L}_T(T)$. This means that equivalence of the timed languages cannot be an admissibility criterion ensuring functional equivalence. At the other end of the spectrum we may relate the de-timed

languages of T and T_ι. The *de-time* operator $\alpha(T)$ is defined such that it omits all timing constraints and resets from any TA T. Requiring $\mathcal{L}(\alpha(T)) = \mathcal{L}(\alpha(T_\iota))$ is tempting since it states that when eliminating all timing related features from T and from the repaired T_ι, the resulting action languages will be identical.

However, this admissibility criterion would be flawed, since the repair in T_ι may imply that unreachable locations in T will be reachable in T_ι, and vice versa. This may have an impact on the untimed languages, and even though $\mathcal{L}(\alpha(T)) = \mathcal{L}(\alpha(T_\iota))$ it may be that $\mathcal{L}_\mu(T) \neq \mathcal{L}_\mu(T_\iota)$. To illustrate this point, consider the running example in Fig. 2 and assume the invariant in location `dbServer.reqReceiving` to be modified from $z \leq 2$ to $z \leq 1$ in the repaired TA T_ι. Applying the de-time operator to T_ι implies that the location `dbServer.timeout`, which is unreachable in T_ι, becomes reachable in the de-timed model. Since `dbServer.timeout` is reachable in T, the TA T and T_ι are not functionally equivalent, even though their de-timed languages are identical. Notice that for the untimed languages $\mathcal{L}_\mu(T) \neq \mathcal{L}_\mu(T_\iota)$ holds since no timed trace in $\mathcal{L}_T(T_\iota)$ reaches location `timeout`, even though such a timed trace exists in $\mathcal{L}_T(T)$. In detail, $\mathcal{L}_\mu(T)$ contains the untimed trace $\Theta_0\Theta_1\Theta_2\Theta_3\Theta_4$ that is missing in $\mathcal{L}_\mu(T_i)$ and where Θ_4 is the transition towards the location `dbServer.timeout`. As consequence, we resort to considering the untimed languages of T and T_ι and require $\mathcal{L}_\mu(T) = \mathcal{L}_\mu(T_\iota)$. It is easy to see that $\mathcal{L}_\mu(T) = \mathcal{L}_\mu(T_\iota) \Rightarrow \mathcal{L}(\alpha(T)) = \mathcal{L}(\alpha(T_\iota))$. In other words, the equivalence of the untimed languages ensures functional equivalence.

Admissibility Test. Designing an algorithmic admissibility test for functional equivalence is challenging due to the computational complexity of determining the equivalence of the untimed languages $\mathcal{L}_\mu(T)$ and $\mathcal{L}_\mu(T_\iota)$. While language equivalence is decidable for languages defined by Büchi Automata, it is undecidable for timed languages [3]. For untimed languages, however, this problem is again decidable [3]. The algorithmic implementation of the test for functional equivalence that we propose proceeds in two steps.

- First, the untimed languages $\mathcal{L}_\mu(T)$ and $\mathcal{L}_\mu(T_\iota)$ are constructed. This requires an untime transformation of T and T_ι yielding Büchi automata representing $\mathcal{L}_\mu(T)$ and $\mathcal{L}_\mu(T_\iota)$. While the standard untime transformation for TAs [3] relies on a region construction, we propose a transformation that relies on a zone construction [14]. This will provide a more succinct representation of the resulting untimed languages and, hence, a more efficient equivalence test.
- Second, it needs to be determined whether $\mathcal{L}_\mu(T) = \mathcal{L}_\mu(T_\iota)$. As we shall see, the obtained Büchi automata are closed. Hence, we can reduce the equivalence problem for these ω-regular languages to checking equivalence of the regular languages obtained by taking the finite prefixes of the traces in $\mathcal{L}_\mu(T)$ and $\mathcal{L}_\mu(T_\iota)$. This allows us to interpret the Büchi automata obtained in the first step as NFAs, for which the language equivalence check is a standard construction [15].

Automata for Untimed Languages. The construction of an automaton representing an untimed language, here referred to as an *untime construction*, has so far been proposed based on a region abstraction [3]. The region abstraction is known to be relatively inefficient since the number of regions is, among other things, exponential in the number of

clocks [4]. We therefore propose an untime construction based on the construction of a zone automaton [14] which in the worst case is of the same complexity as the region automaton, but on the average is more succinct [7].

Definition 3 (Untimed Büchi Automaton). *Assume a TA T and the corresponding zone automaton $[\![T]\!]_Z = (S_Z, s_Z^0, \Sigma_Z, \Theta_Z)$. We define the* untimed Büchi automaton *as the closed BA $B_T = (S, \Sigma, \rightarrow, S_0, F)$ obtained from $[\![T]\!]_Z$ such that $S = S_Z$, $\Sigma = \Sigma_Z \setminus \{\delta\}$ and $S_0 = \{s_Z^0\}$. For every transition in Θ_Z with a label $a \in \Sigma$ we add a transition to $\rightarrow$ created by the rule $\frac{(l,z)\overset{\delta}{\rightsquigarrow}(l,z^\uparrow)\overset{a}{\rightsquigarrow}(l',z')}{(l,z)\overset{a}{\rightarrow}(l',z')}$ with $z^\uparrow = \{v + d | v \in z, d \in \mathbb{R}_{\geq 0}\}$. In addition, we add self-transitions $(l,z) \overset{\tau}{\rightarrow} (l,z)$ to every state $(l,z) \in S_B$.*

The following observations justify this definition:

- A timed trace of T may remain forever in the same location after a finite number of action transitions. In order to enable B to accept this trace, we add a self-transition labeled with τ to $\rightarrow$ for each state $s \in S$ in B_T, and later define s as accepting. These τ-self-transitions extend every finite timed trace t leading to a state in S_τ to an infinite trace $t.\tau^\omega$.
- The construction of the acceptance set F is more intricate. Convergent traces are often excluded from consideration in real-time model checking [4]. As a consequence, in the untime construction proposed in [3], only a subset of the states in S may be included in F. A repair may render a subgraph of the location graph of T that is only reachable by divergent traces, into a subgraph in T_ι that is only reachable by convergent traces. However, excluding convergent traces is only meaningful when considering unbounded liveness properties, but not when analyzing timed safety properties, which in effect are safety properties. As argued in [7], unbounded liveness properties appear to be less important than timed safety properties in timed systems. This is due to the observation that divergent traces reflect unrealistic behavior in the limit, but finite prefixes of infinite divergent traces, which only need to be considered for timed safety properties, correspond to realistic behavior. This observation is also reflected in the way in which, e.g., UPPAAL treats reachability by convergent traces. In conclusion, this justifies our choice to define the zone automaton in the untime construction as a closed BA, i.e., $F = S$.

Theorem 2 (Correctness of Untimed Büchi Automaton Construction). *For an untimed Büchi automaton B_T derived from a TA T according to Definition 3 it holds that $\mathcal{L}(B_T) = \mathcal{L}_\mu(T)$.*

Equivalence Check for Untimed Languages. Given that the zone automaton construction delivers closed BAs we can reduce the admissibility test $\mathcal{L}_\mu(T) = \mathcal{L}_\mu(T_\iota)$ defined over infinite languages to an equivalence test over the finite prefixes of these languages, represented by interpreting the zone automata as NFAs. The following theorem justifies this reduction.

Theorem 3 (Language Equivalence of Closed BA). *Given closed Büchi automata B and B', if $\mathcal{L}_\mathrm{f}(B) = \mathcal{L}_\mathrm{f}(B')$ then $\mathcal{L}(B) = \mathcal{L}(B')$.*

Discussion. One may want to adapt the admissibility test so that it only considers divergent traces, e.g., in cases where only unbounded liveness properties need to be preserved by a repair. This can be accomplished as follows. First, an overapproximating non-zenoness test [4] can be applied to T and T_i. If it shows non-zenoness, then one knows that the respective TA does not include convergent traces. If this test fails, a more expensive test needs to be developed. It requires a construction of the untimed Büchi automata using the approach from [3], and subsequently a language equivalence test of the untimed languages accepted by the untimed BAs using, for instance, the automata-theoretic constructions proposed in [9].

6 Case Studies and Experimental Evaluation

We have implemented the repair computation and admissibility test in a proof-of-concept tool called TARTAR. We present the architecture of TARTAR and then evaluate the proposed method by applying TARTAR to several case studies.

Tool Architecture. The control loop of TARTAR, depicted in Fig. 3, computes repairs for a given UPPAAL model and a given property Π using the following steps:

1. *Counterexample Creation*. TARTAR calls UPPAAL with parameters to compute and store a shortest symbolic TDT in XML format, in case Π is violated.
2. *Diagnostic Trace Creation*. Parsing the model and the TDT, TARTAR creates $\mathcal{F}_H^{bv} \wedge \mathcal{F}_S^{bv}$ as defined in Sect. 4. Z3 can only solve the MaxSMT problem for quantifier-free linear real arithmetic. Hence, TARTAR first performs a quantifier elimination on the constraints $\forall \delta_j, c_j . \mathcal{T}^{bv} \Rightarrow \Phi$ of $\mathcal{F}_H^{bv}$.
3. *Repair Computation*. Next, TARTAR attempts to compute a repair, by using Z3 to solve the generated quantifier-free MaxSMT instance. In case no solution is found, TARTAR terminates. Otherwise, TARTAR returns the repair that has been computed from the model of the MaxSMT solution.
4. *Admissibility Check*. Using adapted routines provided by the opaal model checker [11], TARTAR checks the admissibility of the computed repair. To do so, TARTAR modifies the constraints of the considered UPPAAL model as indicated by the computed repair. It calls opaal in order to compute the timed transition system (TTS) of the original and the repaired UPPAAL model. TARTAR then checks whether the two TTS have equivalent untimed languages, in which case the repair is admissible. This check is implemented using the library AutomataLib included in the package LearnLib [16],
5. *Iteration*. TARTAR is designed to enumerate all repairs, starting with the minimal ones, in an iterative loop. To accomplish this, at the end of each iteration i a new $\mathcal{V}_{i+1}^{bv}$ is generated by forcing the bound variation variables that were used in the i-th repair to 0. This excludes the repair computed in iteration i from further consideration. Using $\mathcal{V}_{i+1}^{bv}$, TARTAR iterates back to Step 3 to compute another repair.

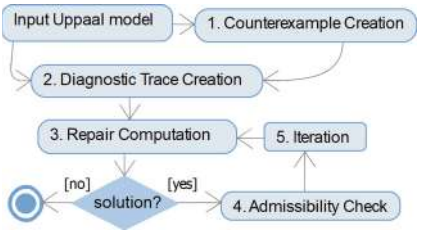


Fig. 3. Control loop of TARTAR

Evaluation Strategy. The evaluation of our analysis is based on ideas taken from mutation testing [18]. Mutation testing evaluates a test set by systematically modifying the program code to be tested and computing the ratio of modifications that are detected by the test set. Real-time system models that contain violations of timed safety properties are not available in significant numbers. We therefore need to seed faults in existing models and check whether those can be found by our automated repair. An objective of mutation testing is that testing a proportion of the possible modification yields satisfactory results [18]. In order to evaluate repairs for erroneous clock bounds in invariants and transition guards we seed modifications to all bounds of clock constraints by the amount of $\{-10, -1, +1, +0.1{\cdot}M, +M\}$, where M is the maximal bound a clock is compared against in a given model. If a thus seeded modification leads to a syntactically invalid UPPAAL model, then UPPAAL returns an exception and we ignore this modification. In analogy to mutation testing, we compute the count of TDTs for which our analysis finds an admissible repair.

Experiments. We have applied this modification seeding strategy to eight UPPAAL models (see Table 1). Not all of the models that we considered have been published with a property that can be violated by mutating a clock constraint. For those models, we suggest a suitable timed safety property specifying an invariant condition. In particular, we add a property to the Bando [29] model which ensures that, for as long as the sender is active, its clock never exceeds the value of 28,116 time units. In the FDDI token ring protocol [29], the property that we use checks whether the first member of the ring never remains for more than 140 time units in any given state. The Viking model is taken from the set of test models of opaal [26]. For this model we use a property that checks whether one of the Viking processes can only enter a safe state during the first 60 time units. Note that all of these properties are satisfied by the unmodified models.

The results of the clock bound repair computed by TARTAR for all considered models are summarized in Table 1. The seeded modifications are characterized quantitatively by the count *#Seed* of analyzed modified models, the count *#TDT* of modified models that return a TDT for the considered property, the maximal time T_{UP} UPPAAL needs to create a TDT per analyzed model, and the length *Len.* of the longest TDT found. For the computation of a repair we give the count *#Rep.* of all repairs that were computed, the count *#Adm.* of computed admissible repairs, the count of TDTs *#Sol.* for which an admissible repair was found, the maximal time T_{QE} that the quantifier elimination required, the average time effort T_R to compute a repair, the standard deviation SD_R for the computation time of a repair, the time effort T_{Adm} for an admissibility check, the maximal count of variables *#Var*, and the maximal count of constraints *#Con.* used in $\mathcal{V}^{bv}_{i+1}$. The maximal memory consumption was at most 17MB for the repair analysis and 478MB for the admissibility test. We performed all experiments on a computer with an i7-6700K CPU (4.0GHz), 60 GB of RAM and a Linux operating system.

We found 60 TDTs by seeding violations of the timed safety property and TARTAR returned 204 repairs for these TDTs. TARTAR proposed an admissible repair for 55 (91%) TDTs and at least one repair for 57 (95%) TDTs. For 3 out of the total of 14 TDTs found for the SBR model no repair was computed since the timeout of the quantifier elimination was reached after 2 minutes. For all other models, no timeout occurred.

Space limitations do not permit us to describe all models and computed repairs in detail, we therefore focus on the pacemaker case study. One of the modification increases a location invariant of this model that controls the minimal heart period from 400 to 1,600. The modification allows the pacemaker to delay an induced ventricular beat for too long so that this violates the property that the time between two ventricular beats of a heart is never longer than the maximal heart period of 1,000. TARTAR finds three repairs. Two repairs reduce the maximal time delay between two ventricular or articular heart beats of the patient. The repairs are classified as inadmissible. In the model context this appears to be reasonable since the repairs would restrict the environment of the pacemaker, and not the pacemaker itself. The third repair is admissible and reduces the bound modified during the seeding of bound modifications by 600.5. The minimal heart period is then below or equal to the maximal heart period of $1,000$.

Result Interpretation. Our repair strategy minimizes the number of repairs but does not optimize the computed value. For instance, in the pacemaker model the computed repair of 600.5 would be a correct and admissible repair even if the value was reduced to 600, which would be the minimal possible repair value.

A comparison of the values T_{QE} and T_R reveals that, perhaps unsurprisingly, the quantifier elimination step is computationally almost an order of magnitude more expensive than the repair computation. Overall, the computational cost ($T_{QE} + T_R$) correlates with the number of variables in the constraint system, which depends in turn on the length of the TDT and the number of clocks referenced along the TDT. Consider, for instance, that the pacemaker model has a TDT of maximal length 9 with 116 variables, and the repair requires 0.193 s and 2.070 MB. On the other hand, the Bando model produces a longer maximal TDT of length 279 with 1,156 variables and requires 6.555 s and 16.650 MB. The impact of the number of clock constraints and clock variables on the computation costs can be seen, for instance, in the data for the pacemaker and FDDI models. While the pacemaker model has a shorter TDT than the Viking model (9 vs. 18), the constraint counts (294 vs. 140) of the pacemaker model are higher than for

Table 1. Experimental results for clock bound repair computation using TARTAR

Model	*# Seed*	# TDT	T_{UP}	*Len.*	*# Rep.*	*# Adm.*	*# Sol.*	T_{QE}	T_R	SD_R	T_{Adm}	*# Var.*	*# Con.*
Repaired db Fig. 2	35	6	0.006 s	4	12	12	6	0.042 s	0.023 s	0.001	2.329 s	25	40
CSMA/CD [17]	90	6	0.012 s	2	36	16	6	0.020 s	0.021 s	0.000	3.060 s	16	36
Elevator [8]	35	3	0.004 s	1	6	6	3	0.071 s	0.028 s	0.005	2.374 s	6	16
Viking	85	3	0.009 s	18	6	6	3	0.032 s	0.042 s	0.002	2.821 s	120	140
Bando [29]	740	12	0.259 s	279	26	24	12	17.227 s	6.555 s	1.776	4.067 s	1,156	2,441
Pacemaker [19]	240	7	0.044 s	9	34	16	7	0.670 s	0.193 s	0.021	3.389 s	116	294
SBR [23]	65	14	0.066 s	81	42	26	9	20.776 s	2.568 s	0.441	34.120 s	256	410
FDDI [29]	100	9	0.025 s	5	42	30	9	0.046 s	0.029 s	0.001	2.493 s	59	93

the Viking model, which coincides with a higher computation time (0.193 s vs. 0.042 s) and a higher memory consumption (2.070 MB vs. 0.910 MB) compared to the Viking model.

We analyzed for every TDT the relationship between the length of the TDT and the computation time for a repair ($T_r = T_{QE} + T_R$), as well as the relationship between *#Var* and T_r by estimating Kendall's tau [13]. Kendall's tau is a measurement for the ordinal association between two measured quantities. A correlation is considered significant if the probability p that there is actually no correlation in a larger data set is below a certain threshold. The length of a TDT is significantly related ($\tau_1 = 0.673$, $p < .001$) to T_r. Also *#Var* is significantly related ($\tau_2 = 0.759$, $p < .001$) to T_r. *#Var* contains clocks for every step of a TDT, hence the combination of trace length and clock count tends to correlate higher than the trace length on its own. This supports our conjecture that the computation time of a repair depends on the trace length and the clock count.

The admissibility test appears to be quite efficient, with a maximum computation time of 34.120 s for the SBR model, which is one of the more complex models that were considered. We observed that most models were action-deterministic, which has a positive influence on the language equivalence test used during admissibility checking.

7 Conclusion

We have presented an approach to derive minimal repairs for timed reachability properties of TA and NTA models from TDTs in order to facilitate fault localization and debugging of such models during the design process. Our approach includes a formalization of TDTs using linear real arithmetic, a repair strategy based on MaxSMT solving, the definition of an admissibility criterion and test for the computed repairs, the development of a prototypical analysis and repair tool, and the application of the proposed method to a number of case studies of realistic complexity. To the best of our knowledge, this is the first rigorous treatment of counterexamples in real-time model checking. We are also not aware of any existing repair approaches for TA or NTA models. This makes a comparative experimental evaluation impossible. We have nonetheless observed that our analysis computes a significant number of admissible repairs within realistic computation time bounds and memory consumption.

Future research will address the development and implementation of repair strategies for further syntactic features in TAs and NTAs, including false comparison operators in invariants and guards, erroneous clock variable references, superfluous or missing resets for clocks, and wrong urgent state choices. We will furthermore address the interplay between different repairs and develop refined strategies to determine their admissibility. Finally, we plan to extend the approach developed in this paper to derive criteria for the actual causation of timing property violations in NTA models based on the counterfactual reasoning paradigm for causation.

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Verifying Asynchronous Interactions via Communicating Session Automata

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Abstract. This paper proposes a sound procedure to verify properties of communicating session automata (CSA), i.e., communicating automata that include multiparty session types. We introduce a new *asynchronous* compatibility property for CSA, called k-multiparty compatibility (k-MC), which is a strict superset of the synchronous multiparty compatibility used in theories and tools based on session types. It is decomposed into two bounded properties: (*i*) a condition called *k-safety* which guarantees that, within the bound, all sent messages can be received and each automaton can make a move; and (*ii*) a condition called *k-exhaustivity* which guarantees that all k-reachable send actions can be fired within the bound. We show that k-exhaustivity implies existential boundedness, and *soundly and completely* characterises systems where each automaton behaves equivalently under bounds greater than or equal to k. We show that checking k-MC is PSPACE-complete, and demonstrate its scalability empirically over large systems (using partial order reduction).

1 Introduction

Communicating automata are a Turing-complete model of asynchronous interactions [10] that has become one of the most prominent for studying point-to-point communications over unbounded first-in-first-out channels. This paper focuses on a class of communicating automata, called *communicating session automata* (CSA), which strictly includes automata corresponding to *asynchronous multiparty session types* [28]. Session types originated as a typing discipline for the π-calculus [27,66], where a session type dictates the behaviour of a process wrt. its communications. Session types and related theories have been applied to the verification and specification of concurrent and distributed systems through their integration in several mainstream programming languages, e.g., Haskell [44,55], Erlang [49], F♯ [48], Go [11,37,38,51], Java [30,31,34,65], OCaml [56], C [52], Python [16,47,50], Rust [32], and Scala [61,62]. Communicating automata and asynchronous multiparty session types [28] are closely related: the latter can be seen as a syntactical representation of the former [17] where a sending state corresponds to an internal choice and a receiving state to an external choice. This

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correspondence between communicating automata and multiparty session types has become the foundation of many tools centred on session types, e.g., for generating communication API from multiparty session (global) types [30,31,48,61], for detecting deadlocks in message-passing programs [51,67], and for monitoring session-enabled programs [5,16,47,49,50]. These tools rely on a property called *multiparty compatibility* [6,18,39], which guarantees that communicating automata representing session types interact correctly, hence enabling the identification of correct protocols or the detection of errors in endpoint programs. Multiparty compatible communicating automata validate two essential requirements for session types frameworks: every message that is sent can be eventually received and each automaton can always eventually make a move. Thus, they satisfy the *abstract* safety invariant φ for session types from [63], a prerequisite for session type systems to guarantee safety of the typed processes. Unfortunately, multiparty compatibility suffers from a severe limitation: it requires that each execution of the system has a synchronous equivalent. Hence, it rules out many correct systems. Hereafter, we refer to this property as *synchronous multiparty compatibility* (SMC) and explain its main limitation with Example 1.

Example 1. The system in Fig. 1 contains an interaction pattern that is *not* supported by any definition of SMC [6,18,39]. It consists of a client (`c`), a server (`s`), and a logger (`l`), which communicate via unbounded FIFO channels. Transition $\texttt{sr}!a$ denotes that `s`ender puts (asynchronously) message a on channel `sr`; and transition $\texttt{sr}?a$ denotes the consumption of a from channel `sr` by `r`eceiver. The `c`lient sends a *req*uest and some *data* in a fire-and-forget fashion, before waiting for a response from the `s`erver. Because of the presence of this simple pattern, the system cannot be executed synchronously (i.e., with the restriction that a send action can only be fired when a matching receive is enabled), hence it is rejected by all definitions of SMC from previous works, even though the system is safe (all sent messages are received and no automaton gets stuck).

Synchronous multiparty compatibility is reminiscent of a strong form of existential boundedness. Among the existing sub-classes of communicating automata (see [46] for a survey), existentially k-bounded communicating automata [22] stand out because they can be model-checked [8,21] and they restrict the model in a natural way: any execution can be rescheduled such that the number of pending messages *that can be received* is bounded by k. However, existential boundedness is generally *undecidable* [22], even for a fixed bound k. This shortcoming makes it impossible to know when theoretical results are applicable.

To address the limitation of SMC and the shortcoming of existential boundedness, we propose a (decidable) sufficient condition for existential boundedness, called *k-exhaustivity*, which serves as a basis for a wider notion of new compatibility, called *k-multiparty compatibility* (k-MC) where $k \in \mathbb{N}_{>0}$ is a bound on the number of pending messages in each channel. A system is k-MC when it is (*i*) *k-exhaustive*, i.e., all k-reachable send actions are enabled within the bound, and (*ii*) *k-safe*, i.e., within the bound k, all sent messages can be received and each automaton can always eventually progress. For example, the system in Fig. 1 is k-multiparty compatible for any $k \in \mathbb{N}_{>0}$, hence it does not lead to communication

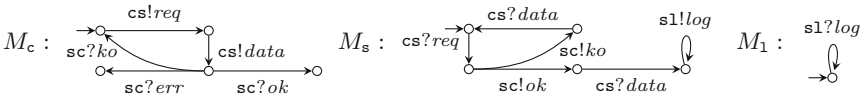


Fig. 1. Client-Server-Logger example.

errors, see Theorem 1. The k-MC condition is a natural constraint for real-world systems. Indeed any finite-state system is k-exhaustive (for k sufficiently large), while any system that is not k-exhaustive (resp. k-safe) for any k is unlikely to work correctly. Furthermore, we show that if a system of CSA validates k-exhaustivity, then each automaton locally behaves equivalently under any bound greater than or equal to k, a property that we call *local bound-agnosticity*. We give a *sound and complete* characterisation of k-exhaustivity for CSA in terms of local bound-agnosticity, see Theorem 3. Additionally, we show that the complexity of checking k-MC is PSPACE-complete (i.e., no higher than related algorithms) and we demonstrate empirically that its cost can be mitigated through (sound and complete) partial order reduction.

In this paper, we consider *communicating session automata* (CSA), which cover the most common form of asynchronous multiparty session types [15] (see *Remark* 3), and have been used as a basis to study properties and extensions of session types [6,7,18,30,31,41,42,47,49,50]. More precisely, CSA are deterministic automata, whose every state is either sending (internal choice), receiving (external choice), or final. We focus on CSA that preserve the intent of internal and external choices from session types. In these CSA, whenever an automaton is in a sending state, it can fire any transition, no matter whether channels are bounded; when it is in a receiving state then at most one action must be enabled.

Synopsis. In Sect. 2, we give the necessary background on communicating automata and their properties, and introduce the notions of output/input bound independence which guarantee that internal/external choices are preserved in bounded semantics. In Sect. 3, we introduce the definition of k-multiparty compatibility (k-MC) and show that k-MC systems are safe for systems which validate the bound independence properties. In Sect. 4, we formally relate existential boundedness [22,35], synchronisability [9], and k-exhaustivity. In Sect. 5 we present an implementation (using partial order reduction) and an experimental evaluation of our theory. We discuss related works in Sect. 6 and conclude in Sect. 7.

See [43] for a full version of this paper (including proofs and additional examples). Our implementation and benchmark data are available online [33].

2 Communicating Automata and Bound Independence

This section introduces notations and definitions of communicating automata (following [12,39]), as well as the notion of output (resp. input) bound independence which enforces the intent of internal (resp. external) choice in CSA.

Fix a finite set $\mathcal{P}$ of *participants* (ranged over by $\mathtt{p}$, $\mathtt{q}$, $\mathtt{r}$, $\mathtt{s}$, etc.) and a finite alphabet Σ. The set of *channels* is $\mathcal{C} \stackrel{\text{def}}{=} \{\mathtt{pq} \mid \mathtt{p},\mathtt{q} \in \mathcal{P} \text{ and } \mathtt{p} \neq \mathtt{q}\}$, $\mathcal{A} \stackrel{\text{def}}{=} \mathcal{C} \times \{!,?\} \times \Sigma$ is the set of *actions* (ranged over by ℓ), Σ^* (resp. $\mathcal{A}^*$) is the set of finite words on Σ (resp. $\mathcal{A}$). Let w range over Σ^*, and ϕ, ψ range over $\mathcal{A}^*$. Also, ϵ ($\notin \Sigma \cup \mathcal{A}$) is the empty word, $|w|$ denotes the length of w, and $w \cdot w'$ is the concatenation of w and w' (these notations are overloaded for words in $\mathcal{A}^*$).

Definition 1 (Communicating automaton). *A* communicating automaton *is a finite transition system given by a triple $M = (Q, q_0, \delta)$ where Q is a finite set of* states*, $q_0 \in Q$ is the initial state, and $\delta \subseteq Q \times \mathcal{A} \times Q$ is a set of* transitions*.*

The transitions of a communicating automaton are labelled by actions in $\mathcal{A}$ of the form $\mathtt{sr}!a$, representing the *emission* of message a from participant $\mathtt{s}$ to $\mathtt{r}$, or $\mathtt{sr}?a$ representing the *reception* of a by $\mathtt{r}$. Define $subj(\mathtt{pq}!a) = subj(\mathtt{qp}?a) = \mathtt{p}$, $obj(\mathtt{pq}!a) = obj(\mathtt{qp}?a) = \mathtt{q}$, and $chan(\mathtt{pq}!a) = chan(\mathtt{pq}?a) = \mathtt{pq}$. The projection of ℓ onto $\mathtt{p}$ is defined as $\pi_{\mathtt{p}}(\ell) = \ell$ if $subj(\ell) = \mathtt{p}$ and $\pi_{\mathtt{p}}(\ell) = \epsilon$ otherwise. Let $\dagger$ range over $\{!,?\}$, we define: $\pi^{\dagger}_{\mathtt{pq}}(\mathtt{pq} \dagger a) = a$ and $\pi^{\dagger'}_{\mathtt{pq}}(\mathtt{sr} \dagger a) = \epsilon$ if either $\mathtt{pq} \neq \mathtt{sr}$ or $\dagger \neq \dagger'$. We extend these definitions to sequences of actions in the natural way.

A state $q \in Q$ with no outgoing transition is *final*; q is *sending* (resp. *receiving*) if it is not final and all its outgoing transitions are labelled by send (resp. receive) actions, and q is *mixed* otherwise. $M = (Q, q_0, \delta)$ is *deterministic* if $\forall (q, \ell, q'), (q, \ell', q'') \in \delta : \ell = \ell' \implies q' = q''$. $M = (Q, q_0, \delta)$ is *send* (resp. *receive*) *directed* if for all sending (resp. receiving) $q \in Q$ and $(q, \ell, q'), (q, \ell', q'') \in \delta : obj(\ell) = obj(\ell')$. M is *directed* if it is send and receive directed.

Remark 1. In this paper, we consider only deterministic communicating automata without mixed states, and call them *Communicating Session Automata* (CSA). We discuss possible extensions of our results beyond this class in Sect. 7.

Definition 2 (System). *Given a communicating automaton $M_{\mathtt{p}} = (Q_{\mathtt{p}}, q_{0\mathtt{p}}, \delta_{\mathtt{p}})$ for each $\mathtt{p} \in \mathcal{P}$, the tuple $S = (M_{\mathtt{p}})_{\mathtt{p} \in \mathcal{P}}$ is a* system*. A* configuration *of S is a pair $s = (\boldsymbol{q}; \boldsymbol{w})$ where $\boldsymbol{q} = (q_{\mathtt{p}})_{\mathtt{p} \in \mathcal{P}}$ with $q_{\mathtt{p}} \in Q_{\mathtt{p}}$ and where $\boldsymbol{w} = (w_{\mathtt{pq}})_{\mathtt{pq} \in \mathcal{C}}$ with $w_{\mathtt{pq}} \in \Sigma^*$; component $\boldsymbol{q}$ is the* control state *and $q_{\mathtt{p}} \in Q_{\mathtt{p}}$ is the* local state *of automaton $M_{\mathtt{p}}$. The* initial configuration *of S is $s_0 = (\boldsymbol{q_0}; \boldsymbol{\epsilon})$ where $\boldsymbol{q_0} = (q_{0\mathtt{p}})_{\mathtt{p} \in \mathcal{P}}$ and we write $\boldsymbol{\epsilon}$ for the $|\mathcal{C}|$-tuple $(\epsilon, \ldots, \epsilon)$.*

Hereafter, we fix a communicating session automaton $M_{\mathtt{p}} = (Q_{\mathtt{p}}, q_{0\mathtt{p}}, \delta_{\mathtt{p}})$ for each $\mathtt{p} \in \mathcal{P}$ and let $S = (M_{\mathtt{p}})_{\mathtt{p} \in \mathcal{P}}$ be the corresponding system whose initial configuration is s_0. For each $\mathtt{p} \in \mathcal{P}$, we assume that $\forall (q, \ell, q') \in \delta_{\mathtt{p}} : subj(\ell) = \mathtt{p}$. We assume that the components of a configuration are named consistently, e.g., for $s' = (\boldsymbol{q'}; \boldsymbol{w'})$, we implicitly assume that $\boldsymbol{q'} = (q'_{\mathtt{p}})_{\mathtt{p} \in \mathcal{P}}$ and $\boldsymbol{w'} = (w'_{\mathtt{pq}})_{\mathtt{pq} \in \mathcal{C}}$.

Definition 3 (Reachable configuration). *Configuration $s' = (\boldsymbol{q'}; \boldsymbol{w'})$ is* reachable *from configuration $s = (\boldsymbol{q}; \boldsymbol{w})$ by* firing transition *ℓ, written $s \xrightarrow{\ell} s'$ (or $s \to s'$ when ℓ is not relevant), if there are $\mathtt{s}, \mathtt{r} \in \mathcal{P}$ and $a \in \Sigma$ such that either:*

1. *(a)* $\ell = \mathtt{sr}!a$ *and* $(q_{\mathtt{s}}, \ell, q'_{\mathtt{s}}) \in \delta_{\mathtt{s}}$, *(b)* $q'_{\mathtt{p}} = q_{\mathtt{p}}$ *for all* $\mathtt{p} \neq \mathtt{s}$, *(c)* $w'_{\mathtt{sr}} = w_{\mathtt{sr}} \cdot a$ *and* $w'_{\mathtt{pq}} = w_{\mathtt{pq}}$ *for all* $\mathtt{pq} \neq \mathtt{sr}$*; or*
2. *(a)* $\ell = \mathtt{sr}?a$ *and* $(q_{\mathtt{r}}, \ell, q'_{\mathtt{r}}) \in \delta_{\mathtt{r}}$, *(b)* $q'_{\mathtt{p}} = q_{\mathtt{p}}$ *for all* $\mathtt{p} \neq \mathtt{r}$, *(c)* $w_{\mathtt{sr}} = a \cdot w'_{\mathtt{sr}}$, *and* $w'_{\mathtt{pq}} = w_{\mathtt{pq}}$ *for all* $\mathtt{pq} \neq \mathtt{sr}$.

Remark 2. Hereafter, we assume that any bound k is finite and $k \in \mathbb{N}_{>0}$.

We write $\rightarrow^*$ for the reflexive and transitive closure of $\rightarrow$. Configuration $(\boldsymbol{q}; \boldsymbol{w})$ is k-bounded if $\forall \mathtt{pq} \in \mathcal{C} : |w_{\mathtt{pq}}| \leqslant k$. We write $s_1 \xrightarrow{\ell_1 \cdots \ell_n} s_{n+1}$ when $s_1 \xrightarrow{\ell_1} s_2 \cdots s_n \xrightarrow{\ell_n} s_{n+1}$, for some $s_2, \ldots, s_n$ (with $n \geqslant 0$); and say that the *execution* $\ell_1 \cdots \ell_n$ is *k-bounded from* s_1 if $\forall 1 \leqslant i \leqslant n+1 : s_i$ is k-bounded. Given $\phi \in \mathcal{A}^*$, we write $\mathtt{p} \notin \phi$ iff $\phi = \phi_0 \cdot \ell \cdot \phi_1 \implies \mathit{subj}(\ell) \neq \mathtt{p}$. We write $s \xrightarrow{\phi}_k s'$ if s' is reachable with a k-bounded execution ϕ from s. The set of *reachable configurations of* S is $RS(S) = \{s \mid s_0 \rightarrow^* s\}$. The *$k$-reachability set of* S is the largest subset $RS_k(S)$ of $RS(S)$ within which each configuration s can be reached by a k-bounded execution from s_0.

Definition 4 streamlines notions of safety from previous works [6,12,18,39] (absence of deadlocks, orphan messages, and unspecified receptions).

Definition 4 (k-Safety). *S is* k-safe *if the following holds* $\forall (\boldsymbol{q}; \boldsymbol{w}) \in RS_k(S)$*:*

(ER) $\forall \mathtt{pq} \in \mathcal{C}$*, if* $w_{\mathtt{pq}} = a \cdot w'$*, then* $(\boldsymbol{q}; \boldsymbol{w}) \rightarrow_k{}^* \xrightarrow{\mathtt{pq}?a}_k$.

(PG) $\forall \mathtt{p} \in \mathcal{P}$*, if* $q_{\mathtt{p}}$ *is* receiving*, then* $(\boldsymbol{q}; \boldsymbol{w}) \rightarrow_k{}^* \xrightarrow{\mathtt{qp}?a}_k$ *for* $\mathtt{q} \in \mathcal{P}$ *and* $a \in \Sigma$.

We say that S is safe *if it validates the unbounded version of k-safety (∞-safe).*

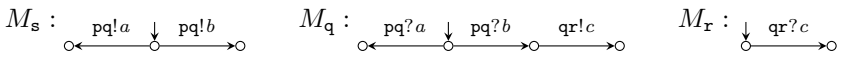
Property (ER), called *eventual reception*, requires that any sent message can always eventually be received (i.e., if a is the head of a queue then there must be an execution that consumes a), and Property (PG), called *progress*, requires that any automaton in a receiving state can eventually make a move (i.e., it can always eventually receive an *expected* message).

We say that a configuration s is *stable* iff $s = (\boldsymbol{q}; \boldsymbol{\epsilon})$, i.e., all its queues are empty. Next, we define the *stable property* for systems of communicating automata, following the definition from [18].

Definition 5 (Stable). *S has the* stable property *(SP) if* $\forall s \in RS(S) : \exists (\boldsymbol{q}; \boldsymbol{\epsilon}) \in RS(S) : s \rightarrow^* (\boldsymbol{q}; \boldsymbol{\epsilon})$.

A system has the stable property if it is possible to reach a stable configuration from any reachable configuration. This property is called *deadlock-free* in [22]. The stable property implies the eventual reception property, but not safety (e.g., an automaton may be waiting for an input in a stable configuration, see Example 2), and safety does not imply the stable property, see Example 4.

Example 2. The following system has the stable property, but it is not safe.



Next, we define two properties related to *bound independence*. They specify classes of CSA whose branching behaviours are not affected by channel bounds.

Definition 6 (k-OBI). *S is k-*output bound independent *(k-OBI), if $\forall s = (\boldsymbol{q}; \boldsymbol{w}) \in RS_k(S)$ and $\forall \mathtt{p} \in \mathcal{P}$, if $s \xrightarrow{\mathtt{pq}!a}_k$, then $\forall (q_{\mathtt{p}}, \mathtt{pr}!b, q'_{\mathtt{p}}) \in \delta_{\mathtt{p}} : s \xrightarrow{\mathtt{pr}!b}_k$.*

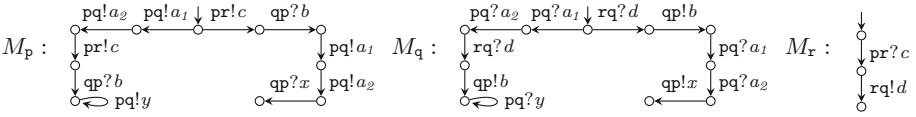


Fig. 2. Example of a *non*-IBI and *non*-safe system.

Definition 7 (k-IBI). *S is k-*input bound independent *(k-IBI), if $\forall s = (\boldsymbol{q}; \boldsymbol{w}) \in RS_k(S)$ and $\forall \mathtt{p} \in \mathcal{P}$, if $s \xrightarrow{\mathtt{qp}?a}_k$, then $\forall \ell \in \mathcal{A} : s \xrightarrow{\ell}_k \wedge subj(\ell) = \mathtt{p} \Longrightarrow \ell = \mathtt{qp}?a$.*

If S is k-OBI, then any automaton that reaches a sending state is able to fire any of its available transitions, i.e., sending states model *internal choices* which are not constrained by bounds greater than or equal to k. Note that the unbounded version of k-OBI ($k = \infty$) is trivially satisfied for any system due to unbounded asynchrony. If S is k-IBI, then any automaton that reaches a receiving state is able to fire at most one transition, i.e., receiving states model *external choices* where the behaviour of the receiving automaton is controlled exclusively by its environment. We write IBI for the unbounded version of k-IBI ($k = \infty$).

Checking the IBI property is generally undecidable. However, systems consisting of (send and receive) *directed* automata are trivially k-IBI and k-OBI for all k, this subclass of CSA was referred to as *basic* in [18]. We introduce larger decidable approximations of IBI with Definitions 10 and 11.

Proposition 1. *(1) If S is send directed, then S is k-OBI for all $k \in \mathbb{N}_{>0}$. (2) If S is receive directed, then S is* IBI *(and k-IBI for all $k \in \mathbb{N}_{>0}$).*

Remark 3. CSA validating k-OBI and IBI strictly include the most common forms of asynchronous multiparty session types, e.g., the directed CSA of [18], and systems obtained by projecting Scribble specifications (global types) which need to be receive directed (this is called "consistent external choice subjects" in [31]) and which validate 1-OBI by construction since they are projections of synchronous specifications where choices must be located at a unique sender.

3 Bounded Compatibility for CSA

In this section, we introduce *k-multiparty compatibility* (k-MC) and study its properties wrt. Safety of communicating session automata (CSA) which are k-OBI and IBI. Then, we soundly and completely characterise k-exhaustivity in terms of local bound-agnosticity, a property which guarantees that communicating automata behave equivalently under any bound greater than or equal to k.

3.1 Multiparty Compatibility

The definition of k-MC is divided in two parts: (*i*) *k-exhaustivity* guarantees that the set of k-reachable configurations contains enough information to make a sound decision wrt. safety of the system; and (*ii*) *k-safety* (Definition 4) guarantees that a subset of all possible executions is free of any communication errors. Next, we define k-exhaustivity, then k-multiparty compatibility. Intuitively, a system is k-exhaustive if for all k-reachable configurations, whenever a send action is enabled, then it can be fired within a k-bounded execution.

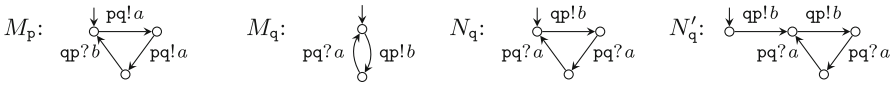


Fig. 3. $(M_{\mathtt{p}}, M_{\mathtt{q}})$ is non-exhaustive, $(M_{\mathtt{p}}, N_{\mathtt{q}})$ is 1-exhaustive, $(M_{\mathtt{p}}, N'_{\mathtt{q}})$ is 2-exhaustive.

Definition 8 (k-Exhaustivity). *S is* k-exhaustive *if* $\forall(\boldsymbol{q};\boldsymbol{w}) \in RS_k(S)$ *and* $\forall \mathtt{p} \in \mathcal{P}$*, if* $q_{\mathtt{p}}$ *is* sending*, then* $\forall(q_{\mathtt{p}}, \ell, q'_{\mathtt{p}}) \in \delta_{\mathtt{p}} : \exists \phi \in \mathcal{A}^* : (\boldsymbol{q};\boldsymbol{w}) \xrightarrow{\phi}_k \xrightarrow{\ell}_k \wedge \mathtt{p} \notin \phi$.

Definition 9 (k-Multiparty compatibility). *S is* k-multiparty compatible *(k-MC) if it is k-safe and k-exhaustive.*

Definition 9 is a natural extension of the definitions of *synchronous* multiparty compatibility given in [18, Definition 4.2] and [6, Definition 4]. The common key requirements are that *every send* action must be matched by a receive action (i.e., send actions are universally quantified), while *at least one receive* action must find a matching send action (i.e., receive actions are existentially quantified). Here, the universal check on send actions is done via the eventual reception property (ER) and the k-exhaustivity condition; while the existential check on receive actions is dealt with by the progress property (PG).

Whenever systems are k-OBI and IBI, then k-exhaustivity implies that k-bounded executions are sufficient to make a sound decision wrt. safety. This is not necessarily the case for systems outside of this class, see Examples 3 and 5.

Example 3. The system $(M_{\mathtt{p}}, M_{\mathtt{q}}, M_{\mathtt{r}})$ in Fig. 2 is k-OBI for any k, but not IBI (it is 1-IBI but not k-IBI for any $k \geqslant 2$). When executing with a bound strictly greater than 1, there is a configuration where $M_{\mathtt{q}}$ is in its initial state and *both* its *receive* transitions are enabled. The system is 1-safe and 1-exhaustive (hence 1-MC) but it is *not* 2-exhaustive nor 2-safe. By constraining the automata to execute with a channel bound of 1, the left branch of $M_{\mathtt{p}}$ is prevented to execute together with the right branch of $M_{\mathtt{q}}$. Thus, the fact that the y messages are not received in this case remains invisible in 1-bounded executions. This example can be easily extended so that it is n-exhaustive (resp. safe) but not $n{+}1$-exhaustive (resp. safe) by sending/receiving $n{+}1$ a_i messages.

Example 4. The system in Fig. 1 is *directed* and 1-MC. The system $(M_{\mathtt{p}}, M_{\mathtt{q}})$ in Fig. 3 is safe but *not* k-MC for any finite $k \in \mathbb{N}_{>0}$. Indeed, for any execution of this system, at least one of the queues grows arbitrarily large. The system $(M_{\mathtt{p}}, N_{\mathtt{q}})$ is 1-MC while the system $(M_{\mathtt{p}}, N'_{\mathtt{q}})$ is *not* 1-MC but it is 2-MC.

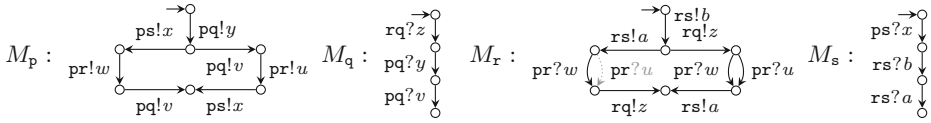


Fig. 4. Example of a system which is not 1-OBI.

Example 5. The system in Fig. 4 (without the dotted transition) is 1-MC, but not 2-safe; it is not 1-OBI but it is 2-OBI. In 1-bounded executions, $M_{\mathtt{r}}$ can execute $\mathtt{rs}!b \cdot \mathtt{rp}!z$, but it cannot fire $\mathtt{rs}!b \cdot \mathtt{rs}!a$ (queue $\mathtt{rs}$ is full), which violates the 1-OBI property. The system with the dotted transition is not 1-OBI, but it is 2-OBI and k-MC for any $k \geqslant 1$. Both systems are receive directed, hence IBI.

Theorem 1. *If S is k-OBI, IBI, and k-MC, then it is safe.*

Remark 4. It is undecidable whether there exists a bound k for which an arbitrary system is k-MC. This is a consequence of the Turing completeness of communicating (session) automata [10,20,42].

Although the IBI property is generally undecidable, it is possible to identify sound approximations, as we show below. We adapt the dependency relation from [39] and say that action ℓ' depends on ℓ from $s = (\boldsymbol{q}; \boldsymbol{w})$, written $s \vdash \ell \prec \ell'$, iff $subj(\ell) = subj(\ell') \vee (chan(\ell) = chan(\ell') \wedge w_{chan(\ell)} = \epsilon)$. Action ℓ' depends on ℓ in ϕ from s, written $s \vdash \ell \prec_\phi \ell'$, if the following holds:

$$s \vdash \ell \prec_\phi \ell' \iff \begin{cases} (s \vdash \ell \prec \ell'' \wedge s \vdash \ell'' \prec_\psi \ell') \vee s \vdash \ell \prec_\psi \ell' & \text{if } \phi = \ell'' \cdot \psi \\ s \vdash \ell \prec \ell' & \text{otherwise} \end{cases}$$

Definition 10. *S is k-*chained input bound independent *(k-CIBI) if $\forall s = (\boldsymbol{q}; \boldsymbol{w}) \in RS_k(S)$ and $\forall \mathtt{p} \in \mathcal{P}$, if $s \xrightarrow{\mathtt{qp}?a}_k s'$, then $\forall (q_{\mathtt{p}}, \mathtt{sp}?b, q'_{\mathtt{p}}) \in \delta_{\mathtt{p}} : \mathtt{s} \neq \mathtt{q} \implies \neg(s \xrightarrow{\mathtt{sp}?b}_k) \wedge (\forall \phi \in \mathcal{A}^* : s' \xrightarrow{\phi}_k \xrightarrow{\mathtt{sp}!b}_k \implies s \vdash \mathtt{qp}?a \prec_\phi \mathtt{sp}!b)$.*

Definition 11. *S is k-*strong input bound independent *(k-SIBI) if $\forall s = (\boldsymbol{q}; \boldsymbol{w}) \in RS_k(S)$ and $\forall \mathtt{p} \in \mathcal{P}$, if $s \xrightarrow{\mathtt{qp}?a}_k s'$, then $\forall (q_{\mathtt{p}}, \mathtt{sp}?b, q'_{\mathtt{p}}) \in \delta_{\mathtt{p}} : \mathtt{s} \neq \mathtt{q} \implies \neg(s \xrightarrow{\mathtt{sp}?b}_k \vee s' \rightarrow^* \xrightarrow{\mathtt{sp}!b}_k)$.*

Definition 10 requires that whenever $\mathtt{p}$ can fire a receive action, at most one of its receive actions is enabled at s, and no other receive transition from $q_{\mathtt{p}}$ will be enabled until $\mathtt{p}$ has made a move. This is due to the existence of a dependency chain between the reception of a message ($\mathtt{qp}?a$) and the matching send of another possible reception ($\mathtt{sp}!b$). Property k-SIBI (Definition 11) is a stronger version of k-CIBI, which can be checked more efficiently.

Lemma 1. *If S is k-OBI, k-CIBI (resp. k-SIBI) and k-exhaustive, then it is* IBI.

The decidability of k-OBI, k-IBI, k-SIBI, k-CIBI, and k-MC is straightforward since both $RS_k(S)$ (which has an exponential number of states wrt. k) and $\rightarrow_k$ are finite, given a finite k. Theorem 2 states the space complexity of the procedures, except for k-CIBI for which a complexity class is yet to be determined. We show that the properties are PSPACE by reducing to an instance of the reachability problem over a transition system built following the construction of Bollig et al. [8, Theorem 6.3]. The rest of the proof follows from similar arguments in Genest et al. [22, Proposition 5.5] and Bouajjani et al. [9, Theorem 3].

Theorem 2. *The problems of checking the k-OBI, k-IBI, k-SIBI, k-safety, and k-exhaustivity properties are all decidable and* PSPACE*-complete (with $k \in \mathbb{N}_{>0}$ given in unary). The problem of checking the k-CIBI property is decidable.*

3.2 Local Bound-Agnosticity

We introduce local bound-agnosticity and show that it fully characterises k-exhaustive systems. Local bound-agnosticity guarantees that each communicating automaton behave in the same manner for any bound greater than or equal to some k. Therefore such systems may be executed transparently under a bounded semantics (a communication model available in Go and Rust).

Definition 12 (Transition system). *The k-bounded transition system of S is the labelled transition system (LTS) $TS_k(S) = (N, s_0, \Delta)$ such that $N = RS_k(S)$, s_0 is the initial configuration of S, $\Delta \subseteq N \times \mathcal{A} \times N$ is the transition relation, and $(s, \ell, s') \in \Delta$ if and only if $s \xrightarrow{\ell}_k s'$.*

Definition 13 (Projection). *Let $\mathcal{T}$ be an LTS over $\mathcal{A}$. The* projection *of $\mathcal{T}$ onto $\mathtt{p}$, written $\pi^{\epsilon}_{\mathtt{p}}(\mathcal{T})$, is obtained by replacing each label ℓ in $\mathcal{T}$ by $\pi_{\mathtt{p}}(\ell)$.*

Recall that the projection of action ℓ, written $\pi_{\mathtt{p}}(\ell)$, is defined in Sect. 2. The automaton $\pi^{\epsilon}_{\mathtt{p}}(TS_k(S))$ is essentially the *local* behaviour of participant $\mathtt{p}$ within the transition system $TS_k(S)$. When each automaton in a system S behaves equivalently for any bound greater than or equal to some k, we say that S is locally bound-agnostic. Formally, S is *locally bound-agnostic for k* when $\pi^{\epsilon}_{\mathtt{p}}(TS_k(S))$ and $\pi^{\epsilon}_{\mathtt{p}}(TS_n(S))$ are weakly bisimilar ($\approx$) for each participant $\mathtt{p}$ and any $n \geqslant k$. For k-OBI and IBI systems, local bound-agnosticity is a *necessary and sufficient* condition for k-exhaustivity, as stated in Theorem 3 and Corollary 1.

Theorem 3. *Let S be a system.*

(1) If $\exists k \in \mathbb{N}_{>0} : \forall \mathtt{p} \in \mathcal{P} : \pi^{\epsilon}_{\mathtt{p}}(TS_k(S)) \approx \pi^{\epsilon}_{\mathtt{p}}(TS_{k+1}(S))$, then S is k-exhaustive.
(2) If S is k-OBI, IBI, and k-exhaustive, then $\forall \mathtt{p} \in \mathcal{P} : \pi^{\epsilon}_{\mathtt{p}}(TS_k(S)) \approx \pi^{\epsilon}_{\mathtt{p}}(TS_{k+1}(S))$.

Corollary 1. *Let S be k-OBI and IBI s.t. $\forall \mathtt{p} \in \mathcal{P} : \pi^{\epsilon}_{\mathtt{p}}(TS_k(S)) \approx \pi^{\epsilon}_{\mathtt{p}}(TS_{k+1}(S))$, then S is locally bound-agnostic for k.*

Theorem 3 (1) is reminiscent of the (PSPACE-complete) checking procedure for existentially bounded systems with the stable property [22] (an *undecidable* property). Recall that k-exhaustivity is not sufficient to guarantee safety, see Examples 3 and 5. We give an effective procedure (based on partial order reduction) to check k-exhaustivity and related properties in [43].

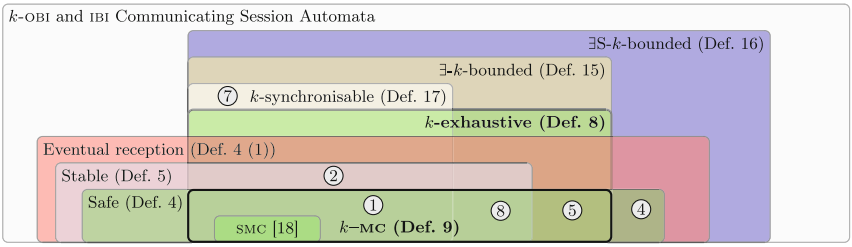


Fig. 5. Relations between k-exhaustivity, existential k-boundedness, and k-synchronisability in k-OBI and IBI CSA (the circled numbers refer to Table 1).

4 Existentially Bounded and Synchronisable Automata

4.1 Kuske and Muscholl's Existential Boundedness

Existentially bounded communicating automata [21,22,35] are a class of communicating automata whose executions can always be scheduled in such a way that the number of pending messages is bounded by a given value. Traditionally, existentially bounded communicating automata are defined on communicating automata that feature (local) accepting states and in terms of *accepting runs*. An accepting run is an execution (starting from s_0) which terminates in a configuration $(\boldsymbol{q}; \boldsymbol{w})$ where each $q_{\mathtt{p}}$ is a local accepting state. In our setting, we simply consider that every local state $q_{\mathtt{p}}$ is an accepting state, hence any execution ϕ starting from s_0 is an accepting run. We first study existential boundedness as defined in [35] as it matches more closely k-exhaustivity, we study the "classical" definition of existential boundedness [22] in Sect. 4.2.

Following [35], we say that an execution $\phi \in \mathcal{A}^*$ is *valid* if for any prefix ψ of ϕ and any channel $\mathtt{pq} \in \mathcal{C}$, we have that $\pi^{?}_{\mathtt{pq}}(\psi)$ is a prefix of $\pi^{!}_{\mathtt{pq}}(\psi)$, i.e., an execution is valid if it models the FIFO semantics of communicating automata.

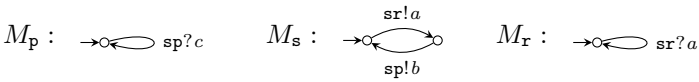
Definition 14 (Causal equivalence [35]). *Given $\phi, \psi \in \mathcal{A}^*$, we define: $\phi \precsim \psi$* iff *ϕ and ψ are* valid *executions and $\forall \mathtt{p} \in \mathcal{P} : \pi_{\mathtt{p}}(\phi) = \pi_{\mathtt{p}}(\psi)$. We write $[\phi]_{\precsim}$ for the equivalence class of ϕ wrt. $\precsim$.*

Definition 15 (Existential boundedness [35]). *We say that a valid execution ϕ is k-*match-bounded *if, for every prefix ψ of ϕ the difference between the number of* matched *events of type* pq! *and those of type* pq? *is bounded by k, i.e., $min\{|\pi^{!}_{\mathtt{pq}}(\psi)|, |\pi^{?}_{\mathtt{pq}}(\phi)|\} - |\pi^{?}_{\mathtt{pq}}(\psi)| \leqslant k$.*
Write $\mathcal{A}^*|_k$ for the set of k-match-bounded words. An execution ϕ is existentially *k-bounded if $[\phi]_{\precsim} \cap \mathcal{A}^*|_k \neq \varnothing$. A system S is existentially k-bounded, written $\exists$-k-bounded, if each execution in $\{\phi \mid \exists s : s_0 \xrightarrow{\phi} s\}$ is existentially k-bounded.*

Example 6. Consider Fig. 3. $(M_{\mathtt{p}}, M_{\mathtt{q}})$ is *not* existentially k-bounded, for any k: at least one of the queues must grow infinitely for the system to progress. Systems $(M_{\mathtt{p}}, N_{\mathtt{q}})$ and $(M_{\mathtt{p}}, N'_{\mathtt{q}})$ are existentially bounded since any of their executions can be scheduled to an $\precsim$-equivalent execution which is 2-match-bounded.

The relationship between k-exhaustivity and existential boundedness is stated in Theorem 4 and illustrated in Fig. 5 for k-OBI and IBI CSA, where SMC refers to synchronous multiparty compatibility [18, Definition 4.2]. The circled numbers in the figure refer to key examples summarised in Table 1. The strict inclusion of k-exhaustivity in existential k-boundedness is due to systems that do not have the eventual reception property, see Example 7.

Example 7. The system below is $\exists$-1-bounded but is *not* k-exhaustive for any k.



For any k, the channel sp eventually gets full and the send action sp!b can no longer be fired; hence it does *not* satisfy k-exhaustivity. Note that each execution can be reordered into a 1-match-bounded execution (the b's are never matched).

Theorem 4. *(1) If S is k-*OBI, IBI, *and k-exhaustive, then it is $\exists$-k-bounded. (2) If S is $\exists$-k-bounded and satisfies eventual reception, then it is k-exhaustive.*

4.2 Existentially Stable Bounded Communicating Automata

The "classical" definition of existentially bounded communicating automata as found in [22] differs slightly from Definition 15, as it relies on a different notion of accepting runs, see [22, page 4]. Assuming that all local states are accepting, we adapt their definition as follows: a *stable accepting run* is an execution ϕ starting from s_0 which terminates in a *stable* configuration.

Definition 16 (Existential stable boundedness [22]). *A system S is* existentially stable k-bounded, *written $\exists S$-k-bounded, if for each execution ϕ in $\{\phi \mid \exists (\boldsymbol{q}; \boldsymbol{\epsilon}) \in RS(S) : s_0 \xrightarrow{\phi} (\boldsymbol{q}; \boldsymbol{\epsilon})\}$ there is ψ such that $s_0 \xrightarrow{\psi}_k$ with $\phi \precsim \psi$.*

A system is existentially stable k-bounded if each of its executions leading to a *stable* configuration can be re-ordered into a k-bounded execution (from s_0).

Theorem 5. *(1) If S is existentially k-bounded, then it is existentially* stable *k-bounded. (2) If S is existentially* stable *k-bounded and has the stable property, then it is existentially k-bounded.*

We illustrate the relationship between existentially stable bounded communicating automata and the other classes in Fig. 5. The example below further illustrates the strictness of the inclusions, see Table 1 for a summary.

Example 8. Consider the systems in Fig. 3. $(M_\mathtt{p}, M_\mathtt{q})$ and $(M_\mathtt{p}, N'_\mathtt{q})$ are (trivially) existentially stable 1-bounded since none of their (non-empty) executions terminate in a stable configuration. The system $(M_\mathtt{p}, N_\mathtt{q})$ is existentially stable 2-bounded since each of its executions can be re-ordered into a 2-bounded one. The system in Example 7 is (trivially) ∃S-1-bounded: none of its (non-empty) executions terminate in a stable configuration (the b's are never received).

Theorem 6. *Let S be an ∃(S)-k-bounded system with the stable property, then it is k-exhaustive.*

Table 1. Properties for key examples, where direct. stands for directed, OBI for k-OBI, SIBI for k-SIBI, ER for eventual reception property, SP for stable property, exh. for k-exhaustive, ∃(S)-b for ∃(S)-bounded, and syn. for n-synchronisable (for some $n \in \mathbb{N}_{>0}$).

#	System	Ref.	k	direct.	OBI	SIBI	safe	ER	SP	exh.	∃S-b	∃-b	syn.
1	$(M_\mathtt{c}, M_\mathtt{s}, M_1)$	Figure 1	1	yes	yes	yes	yes	yes	yes	yes	yes	yes	yes
2	$(M_\mathtt{s}, M_\mathtt{q}, M_\mathtt{r})$	Example 2	1	yes	yes	yes	no	yes	yes	yes	yes	yes	yes
3	$(M_\mathtt{p}, M_\mathtt{q}, M_\mathtt{r})$	Figure 2	$\geqslant 2$	no	yes	no	no	no	no	no	yes	yes	no
4	$(M_\mathtt{p}, M_\mathtt{q})$	Figure 3	any	yes	yes	yes	yes	yes	no	no	yes	no	no
5	$(M_\mathtt{p}, N'_\mathtt{q})$	Figure 3	2	yes	yes	yes	yes	yes	no	yes	yes	yes	no
6	$(M_\mathtt{p}, M_\mathtt{q}, M_\mathtt{r}, M_\mathtt{s})$	Figure 4	2	no	yes	yes	yes	yes	no	yes	yes	yes	no
7	$(M_\mathtt{s}, M_\mathtt{r}, M_\mathtt{p})$	Example 7	any	yes	yes	yes	no	no	no	no	yes	yes	yes
8	$(M_\mathtt{p}, M_\mathtt{q})$	Example 9	1	yes	yes	yes	yes	yes	yes	yes	yes	yes	no

4.3 Synchronisable Communicating Session Automata

In this section, we study the relationship between synchronisability [9] and k-exhaustivity via existential boundedness. Informally, communicating automata are synchronisable if each of their executions can be scheduled in such a way that it consists of sequences of "exchange phases", where each phase consists of a bounded number of send actions, followed by a sequence of receive actions. The original definition of k-synchronisable systems [9, Definition 1] is based on

communicating automata with *mailbox* semantics, i.e., each automaton has one input queue. Here, we adapt the definition so that it matches our point-to-point semantics. We write $\mathcal{A}_!$ for $\mathcal{A} \cap (\mathcal{C} \times \{!\} \times \Sigma)$, and $\mathcal{A}_?$ for $\mathcal{A} \cap (\mathcal{C} \times \{?\} \times \Sigma)$.

Definition 17 (Synchronisability). *A valid execution $\phi = \phi_1 \cdots \phi_n$ is a* k-exchange *if and only if: (1)* $\forall 1 \leqslant i \leqslant n : \phi_i \in \mathcal{A}_!^* \cdot \mathcal{A}_?^* \wedge |\phi_i| \leqslant 2k$*; and (2)* $\forall \mathtt{pq} \in \mathcal{C} : \forall 1 \leqslant i \leqslant n : \pi^!_{\mathtt{pq}}(\phi_i) \neq \pi^?_{\mathtt{pq}}(\phi_i) \implies \forall i < j \leqslant n : \pi^?_{\mathtt{pq}}(\phi_j) = \epsilon$.

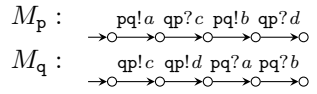
We write $\mathcal{A}^* \|_k$ for the set of executions that are k-exchanges and say that an execution ϕ is k-synchronisable *if $[\phi]_{\precsim} \cap \mathcal{A}^* \|_k \neq \varnothing$. A system S is* k-synchronisable *if each execution in $\{\phi \mid \exists s : s_0 \xrightarrow{\phi} s\}$ is k-synchronisable.*

Table 2. Experimental evaluation. $|\mathcal{P}|$ is the number of participants, k is the bound, $|RTS|$ is the number of transitions in the *reduced* $TS_k(S)$ (see [43]), direct. stands for directed, Time is the time taken to check all the properties shown in this table, and GMC is `yes` if the system is generalised multiparty compatible [39].

Example	$\lvert\mathcal{P}\rvert$	k	$\lvert RTS\rvert$	*direct.*	k-OBI	k-CIBI	k-MC	Time	GMC
Client-Server-Logger	3	1	11	yes	yes	yes	yes	0.04 s	no
4 Player game† [39]	4	1	20	no	yes	yes	yes	0.05 s	yes
Bargain [39]	3	1	8	yes	yes	yes	yes	0.03 s	yes
Filter collaboration [68]	2	1	10	yes	yes	yes	yes	0.03 s	yes
Alternating bit† [59]	2	1	8	yes	yes	yes	yes	0.04 s	no
TPMContract v2† [25]	2	1	14	yes	yes	yes	yes	0.04 s	yes
Sanitary agency† [60]	4	1	34	yes	yes	yes	yes	0.07 s	yes
Logistic† [54]	4	1	26	yes	yes	yes	yes	0.05 s	yes
Cloud system v4 [24]	4	2	16	no	yes	yes	yes	0.04 s	yes
Commit protocol [9]	4	1	12	yes	yes	yes	yes	0.03 s	yes
Elevator† [9]	5	1	72	no	yes	no	yes	0.14s	no
Elevator-dashed† [9]	5	1	80	no	yes	no	yes	0.16s	no
Elevator-directed† [9]	3	1	41	yes	yes	yes	yes	0.07 s	yes
Dev system [58]	4	1	20	yes	yes	yes	yes	0.05 s	no
Fibonacci [48]	2	1	6	yes	yes	yes	yes	0.03 s	yes
SAP-Negot. [48,53]	2	1	18	yes	yes	yes	yes	0.04 s	yes
SH [48]	3	1	30	yes	yes	yes	yes	0.06 s	yes
Travel agency [48,64]	3	1	21	yes	yes	yes	yes	0.05 s	yes
HTTP [29,48]	2	1	48	yes	yes	yes	yes	0.07 s	yes
SMTP [30,48]	2	1	108	yes	yes	yes	yes	0.08 s	yes
gen_server (buggy) [67]	3	1	56	no	no	yes	no	0.03 s	no
gen_server (fixed) [67]	3	1	45	no	yes	yes	yes	0.03 s	yes
Double buffering [45]	3	2	16	yes	yes	yes	yes	0.01 s	no

Condition (1) says that execution ϕ should be a sequence of an arbitrary number of send-receive phases, where each phase consists of at most $2k$ actions. Condition (2) says that if a message is not received in the phase in which it is sent, then it cannot be received in ϕ. Observe that the bound k is on the number of actions (over possibly different channels) in a phase rather than the number of pending messages in a given channel.

Example 9. The system below (left) is 1-MC and ∃(S)-1-bounded, but it is *not* k-synchronisable for any k. The subsequences of send-receive actions in the $\precsim$-equivalent executions below are highlighted (right).



$$\phi_1 = \underbrace{\mathtt{pq}!a}\cdot\underbrace{\mathtt{qp}!c\cdot\mathtt{qp}?c}\cdot\underbrace{\mathtt{qp}!d\cdot\mathtt{pq}?a}\cdot\underbrace{\mathtt{pq}!b\cdot\mathtt{qp}?d\cdot\mathtt{pq}?b}$$

$$\phi_2 = \underbrace{\mathtt{pq}!a\cdot\mathtt{qp}!c\cdot\mathtt{qp}!d\cdot\mathtt{qp}?c\cdot\mathtt{pq}?a}\cdot\underbrace{\mathtt{pq}!b\cdot\mathtt{qp}?d\cdot\mathtt{pq}?b}$$

Execution ϕ_1 is 1-bounded for s_0, but it is not a k-exchange since, e.g., a is received outside of the phase where it is sent. In ϕ_2, message d is received outside of its sending phase. In the terminology of [9], this system is not k-synchronisable because there is a "*receive-send dependency*" between the exchange of message c and b, i.e., $\mathtt{p}$ must receive c before it sends b. Hence, there is no k-exchange that is $\precsim$-equivalent to ϕ_1 and ϕ_2.

Theorem 7. *(1) If S is k-synchronisable, then it is ∃-k-bounded. (2) If S is k-synchronisable and has the eventual reception property, then it is k-exhaustive.*

Figure 5 and Table 1 summarise the results of Sect. 4 wrt. k-OBI and IBI CSA. We note that any finite-state system is k-exhaustive (and ∃(S)-k-bounded) for sufficiently large k, while this does not hold for synchronisability, see Example 9.

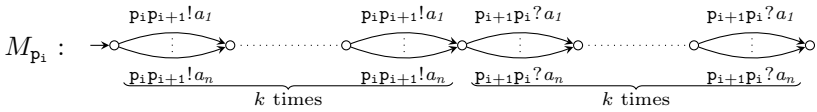
5 Experimental Evaluation

We have implemented our theory in a tool [33] which takes two inputs: (*i*) a system of communicating automata and (*ii*) a bound MAX. The tool iteratively checks whether the system validates the premises of Theorem 1, until it succeeds or reaches k = MAX. We note that the k-OBI and IBI conditions are required for our soundness result (Theorem 1), but are orthogonal for checking k-MC. Each condition is checked on a *reduced bounded transition system*, called $RTS_k(S)$. Each verification procedure for these conditions is implemented in Haskell using a simple (depth-first-search based) reachability check on the paths of $RTS_k(S)$. We give an (optimal) partial order reduction algorithm to construct $RTS_k(S)$ in [43] and show that it preserves our properties.

We have tested our tool on 20 examples taken from the literature, which are reported in Table 2. The table shows that the tool terminates virtually instantaneously on all examples. The table suggests that many systems are indeed k-MC and most can be easily adapted to validate bound independence. The last column refers to the GMC condition, a form of *synchronous* multiparty compatibility (SMC) introduced in [39]. The examples marked with † have been slightly

modified to make them CSA that validate k-OBI and IBI. For instance, we take only one of the possible interleavings between mixed actions to remove mixed states (taking send action before receive action to preserve safety), see [43].

We have assessed the scalability of our approach with automatically generated examples, which we report in Fig. 6. Each system considered in these benchmarks consists of $2m$ (directed) CSA for some $m \geqslant 1$ such that $S = (M_{\mathtt{p}_i})_{1 \leqslant i \leqslant 2m}$, and each automaton $M_{\mathtt{p}_i}$ is of the form (when i is *odd*):



Each $M_{\mathtt{p}_i}$ sends k messages to participant $\mathtt{p}_{i+1}$, then receives k messages from $\mathtt{p}_{i+1}$. Each message is taken from an alphabet $\{a_1, \ldots, a_n\}$ ($n \geqslant 1$). $M_{\mathtt{p}_i}$ has the same structure when i is *even*, but interacts with $\mathtt{p}_{i-1}$ instead. Observe that any system constructed in this way is k-MC for any $k \geqslant 1$, $n \geqslant 1$, and $m \geqslant 1$. The shape of these systems allows us to assess how our approach fares in the worst case, i.e., large number of paths in $RTS_k(S)$. Figure 6 gives the time taken for our tool to terminate (y axis) wrt. the number of transitions in $RTS_k(S)$ where k is the least natural number for which the system is k-MC. The plot on the left in Fig. 6 gives the timings when k is increasing (every increment from $k = 2$ to $k = 100$) with the other parameters fixed ($n = 1$ and $m = 5$). The middle plot gives the timings when m is increasing (every increment from $m = 1$ to $m = 26$) with $k = 10$ and $n = 1$. The right-hand side plot gives the timings when n is increasing (every increment from $n = 1$ to $n = 10$) with $k = 2$ and $m = 1$. The largest $RTS_k(S)$ on which we have tested our tool has 12222 states and 22220 transitions, and the verification took under 17 min.[1] Observe that partial order reduction mitigates the increasing size of the transition system on which k-MC is checked, e.g., these experiments show that parameters k and m have only a linear effect on the number of transitions (see horizontal distances between data points). However the number of transitions increases exponentially with n (since the number of paths in each automaton increases exponentially with n).

6 Related Work

Theory of communicating automata Communicating automata were introduced, and shown to be Turing powerful, in the 1980s [10] and have since then been studied extensively, namely through their connection with message sequence charts (MSC) [46]. Several works achieved decidability results by using bag or lossy channels [1,2,13,14] or by restricting the topology of the network [36,57].

Existentially bounded communicating automata stand out because they preserve the FIFO semantics of communicating automata, do not restrict the topology of the network, and include infinite state systems. Given a bound k and

[1] All the benchmarks in this paper were run on an 8-core Intel i7-7700 machine with 16 GB RAM running a 64-bit Linux.

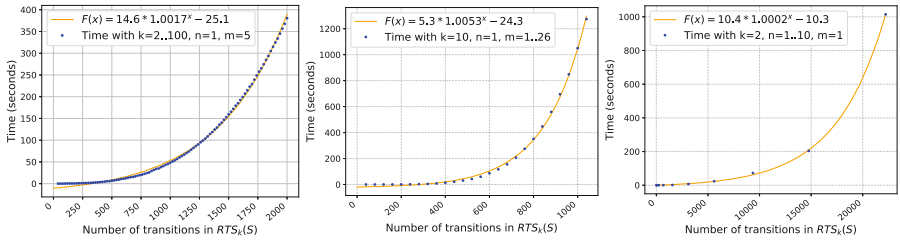


Fig. 6. Benchmarks: increasing k (left), increasing m (middle), and increasing n (right).

an arbitrary system of (deterministic) communicating automata S, it is generally *undecidable* whether S is existentially k-bounded. However, the question becomes decidable (PSPACE-complete) when S has the stable property. The stable property is itself generally *undecidable* (it is called deadlock-freedom in [22,35]). Hence this class is *not* directly applicable to the verification of message passing programs since its membership is overall undecidable. We have shown that k-OBI, IBI, and k-exhaustive CSA systems are (strictly) included in the class of existentially bounded systems. Hence, our work gives a sound *practical* procedure to check whether CSA are existentially k-bounded. To the best of our knowledge, the only tools dedicated to the verification of (unbounded) communicating automata are McScM [26] and Chorgram [40]. Bouajjani et al. [9] study a variation of communicating automata with *mailboxes* (one input queue per automaton). They introduce the class of synchronisable systems and a procedure to check whether a system is k-synchronisable; it relies on executions consisting of k-bounded exchange phases. Given a system and a bound k, it is decidable (PSPACE-complete) whether its executions are equivalent to k-synchronous executions. Section 4.3 states that any k-synchronisable system which satisfies eventual reception is also k-exhaustive, see Theorem 7. In contrast to existential boundedness, synchronisability does not include all finite-state systems. Our characterisation result, based on local bound-agnosticity (Theorem 3), is *unique* to k-exhaustivity. It does not apply to existential boundedness nor synchronisability, see, e.g., Example 7. The term "synchronizability" is used by Basu et al. [3,4] to refer to another verification procedure for communicating automata with mailboxes. Finkel and Lozes [19] have shown that this notion of synchronizability is undecidable. We note that a system that is safe with a point-to-point semantics, may not be safe with a mailbox semantics (due to independent send actions), and vice-versa. For instance, the system in Fig. 2 is safe when executed with mailbox semantics.

Multiparty Compatibility and Programming Languages. The first definition of multiparty compatibility appeared in [18, Definition 4.2], inspired by the work in [23], to characterise the relationship between global types and communicating automata. This definition was later adapted to the setting of communicating timed automata in [6]. Lange et al. [39] introduced a generalised version of multiparty compatibility (GMC) to support communicating automata that feature

mixed or non-directed states. Because our results apply to automata without mixed states, k-MC is not a strict extension of GMC, and GMC is not a strict extension of k-MC either, as it requires the existence of *synchronous* executions. In future work, we plan to develop an algorithm to synthesise representative choreographies from k-MC systems, using the algorithm in [39].

The notion of multiparty compatibility is at the core of recent works that apply session types techniques to programming languages. Multiparty compatibility is used in [51] to detect deadlocks in Go programs, and in [30] to study the well-formedness of Scribble protocols [64] through the compatibility of their projections. These protocols are used to generate various endpoint APIs that implement a Scribble specification [30,31,48], and to produce runtime monitoring tools [47,49,50]. Taylor et al. [67] use multiparty compatibility and choreography synthesis [39] to automate the analysis of the `gen_server` library of Erlang/OTP. We can transparently widen the set of safe programs captured by these tools by using k-MC instead of synchronous multiparty compatibility (SMC). The k-MC condition corresponds to a much wider instance of the *abstract* safety invariant φ for session types defined in [63]. Indeed k-MC includes SMC (see [43]) and all finite-state systems (for k sufficiently large).

7 Conclusions

We have studied CSA via a new condition called k-exhaustivity. The k-exhaustivity condition is (*i*) the basis for a wider notion of multiparty compatibility, k-MC, which captures asynchronous interactions and (*ii*) the first practical, empirically validated, sufficient condition for existential k-boundedness. We have shown that k-exhaustive systems are fully characterised by local bound-agnosticity (each automaton behaves equivalently for any bound greater than or equal to k). This is a key requirement for asynchronous message passing programming languages where the possibility of having infinitely many orphan messages is undesirable, in particular for Go and Rust which provide *bounded* communication channels.

For future work, we plan to extend our theory beyond CSA. We believe that it is possible to support mixed states and states which do not satisfy IBI, as long as their outgoing transitions are independent (i.e., if they commute). Additionally, to make k-MC checking more efficient, we will elaborate heuristics to find optimal bounds and off-load the verification of k-MC to an off-the-shelf model checker.

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Security and Hyperproperties

Verifying Hyperliveness

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Abstract. HyperLTL is an extension of linear-time temporal logic for the specification of hyperproperties, i.e., temporal properties that relate multiple computation traces. HyperLTL can express information flow policies as well as properties like symmetry in mutual exclusion algorithms or Hamming distances in error-resistant transmission protocols. Previous work on HyperLTL model checking has focussed on the alternation-free fragment of HyperLTL, where verification reduces to checking a standard trace property over an appropriate self-composition of the system. The alternation-free fragment does, however, not cover general hyperliveness properties. Universal formulas, for example, cannot express the secrecy requirement that for every possible value of a secret variable there exists a computation where the value is different while the observations made by the external observer are the same. In this paper, we study the more difficult case of hyperliveness properties expressed as HyperLTL formulas with quantifier alternation. We reduce existential quantification to strategic choice and show that synthesis algorithms can be used to eliminate the existential quantifiers automatically. We furthermore show that this approach can be extended to reactive system synthesis, i.e., to automatically construct a reactive system that is guaranteed to satisfy a given HyperLTL formula.

1 Introduction

HyperLTL [6] is a temporal logic for *hyperproperties* [7], i.e., for properties that relate multiple computation traces. Hyperproperties cannot be expressed in standard linear-time temporal logic (LTL), because LTL can only express *trace properties*, i.e., properties that characterize the correctness of individual computations. Even branching-time temporal logics like CTL and CTL*, which quantify

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over computation paths, cannot express hyperproperties, because quantifying over a second path automatically means that the subformula can no longer refer to the previously quantified path. HyperLTL addresses this limitation with quantifiers over trace variables, which allow the subformula to refer to all previously chosen traces. For example, *noninterference* [21] between a secret input h and a public output o can be specified in HyperLTL by requiring that all pairs of traces π and π' that always have the same inputs except for h (i.e., all inputs in $I \setminus \{h\}$ are equal on π and π') also have the same output o at all times:

$$\forall \pi . \forall \pi' .\ \square \Big(\bigwedge_{i \in I \setminus \{h\}} i_\pi = i_{\pi'} \Big) \ \Rightarrow\ \square (o_\pi = o_{\pi'})$$

This formula states that a change in the secret input h alone cannot cause any difference in the output o.

For certain properties of interest, the additional expressiveness of HyperLTL comes at no extra cost when considering the model checking problem. To check a property like noninterference, which only has universal trace quantifiers, one simply builds the self-composition of the system, which provides a separate copy of the state variables for each trace. Instead of quantifying over all pairs of traces, it then suffices to quantify over individual traces of the self-composed system, which can be done with standard LTL. Model checking universal formulas is NLOGSPACE-complete in the size of the system and PSPACE-complete in the size of the formula, which is precisely the same complexity as for LTL.

Universal HyperLTL formulas suffice to express hypersafety properties like noninterference, but not hyperliveness properties that require, in general, quantifier alternation. A prominent example is *generalized noninterference* (GNI) [27], which can be expressed as the following HyperLTL formula:

$$\forall \pi . \forall \pi' . \exists \pi'' .\ \square (h_\pi = h_{\pi''}) \ \wedge\ \square (o_{\pi'} = o_{\pi''})$$

This formula requires that for every pair of traces π and π', there is a third trace π'' in the system that agrees with π on h and with π' on o. The existence of an appropriate trace π'' ensures that in π and π', the value of o is not determined by the value of h. Generalized noninterference stipulates that low-security outputs may not be altered by the injection of high-security inputs, while permitting nondeterminism in the low-observable behavior. The existential quantifier is needed to allow this nondeterminism. GNI is a hyperliveness property [7] even though the underlying LTL formula is a safety property. The reason for that is that we can extend any set of traces that violates GNI into a set of traces that satisfies GNI, by adding, for each offending pair of traces π, π', an appropriate trace π''.

Hyperliveness properties also play an important role in applications beyond security. For example, *robust cleanness* [9] specifies that significant differences in the output behavior are only permitted after significant differences in the input:

$$\forall \pi . \forall \pi' . \exists \pi'' .\ \square \big(i_{\pi'} = i_{\pi''}\big) \ \wedge\ \big(\hat{d}(o_\pi, o_{\pi''}) \leq \kappa_o \ \mathcal{W}\ \hat{d}(i_\pi, i_{\pi''}) > \kappa_i\big)$$

The differences are measured by a distance function $\hat{d}$ and compared to constant thresholds κ_i for the input and κ_o for the output. The formula specifies

the existence of a trace π'' that globally agrees with π' on the input and where the difference in the output o between π and π'' is bounded by κ_o, unless the difference in the input i between π and π'' was greater than κ_i. Robust cleanness, thus, forbids unexpected jumps in the system behavior that are, for example, due to software doping, while allowing for behavioral differences due to nondeterminism.

With quantifier alternation, the model checking problem becomes much more difficult. Model checking HyperLTL formulas of the form $\forall^*\exists^*\varphi$, where φ is a quantifier-free formula, is PSPACE-complete in the size of the system and EXPSPACE-complete in the formula. The only known model checking algorithm replaces the existential quantifier with the negation of a universal quantifier over the negated subformula; but this requires a complementation of the system behavior, which is completely impractical for realistic systems.

In this paper, we present an alternative approach to the verification of hyperliveness properties. We view the model checking problem of a formula of the form $\forall\pi.\exists\pi'.\ \varphi$ as a game between the $\forall$-player and the $\exists$-player. While the $\forall$-player moves through the state space of the system building trace π, the $\exists$-player must match each move in a separate traversal of the state space resulting in a trace π' such that the pair π, π' satisfies φ. Clearly, the existence of a winning strategy for the $\exists$-player implies that $\forall\pi.\exists\pi'.\ \varphi$ is satisfied. The converse is not necessarily true: Even if there always is a trace π' that matches the universally chosen trace π, the $\exists$-player may not be able to construct this trace, because she only knows about the choices made by the $\forall$-player in the finite prefix of π that has occurred so far, and not the choices that will be made by the $\forall$-player in the infinite future. We address this problem by introducing *prophecy variables* into the system. Without changing the behavior of the system, the prophecy variables give the $\exists$-player the information about the future that is needed to make the right choice after seeing only the finite prefix. Such prophecy variables can be provided manually by the user of the model checker to provide a lookahead on future moves of the $\forall$-player.

This game-theoretic approach provides an opportunity for the user to reduce the complexity of the model checking problem: If the user provides a strategy for the $\exists$-player, then the problem reduces to the cheaper model checking problem for universal properties. We show that such strategies can also be constructed automatically using synthesis. Beyond model checking, the game-theoretic approach also provides a method for the synthesis of systems that satisfy a conjunction of hypersafety and hyperliveness properties. Here, we do not only synthesize the strategy, but also construct the system itself, i.e., the game graph on which the model checking game is played. While the synthesis from $\forall^*\exists^*$ hyperproperties is known to be undecidable in general, we show that the game-theoretic approach can naturally be integrated into bounded synthesis, which checks for the existence of a correct system up to a bound on the number of states.

Related Work. While the verification of general HyperLTL formulas has been studied before [6,17,18], there has been, so far, no practical model checking algorithm for HyperLTL formulas with quantifier alternation. The existing algorithm involves a complementation of the system automaton, which results in an

exponential blow-up of the state space [18]. The only existing model checker for HyperLTL, MCHyper [18], was therefore, so far, limited to the alternation-free fragment. Although some hyperliveness properties lie in this fragment, quantifier alternation is needed to express general hyperliveness properties like GNI. In this paper, we present a technique to model check these hyperliveness properties and extend MCHyper to formulas with quantifier alternation.

The situation is similar in the area of reactive synthesis. There is a synthesis algorithm that automatically constructs implementations from HyperLTL specifications [13] using the bounded synthesis approach [20]. This algorithm is, however, also only applicable to the alternation-free fragment of HyperLTL. In this paper, we extend the bounded synthesis approach to HyperLTL formulas with quantifier alternation. Beyond the model checking and synthesis problems, the satisfiability [11,12,14] and monitoring [15,16,22] problems of HyperLTL have also been studied in the past.

For certain information-flow security policies, there are verification techniques that use methods related to our model checking and synthesis algorithms. Specifically, the self-composition technique [2,3], a construction based on the product of copies of a system, has been tailored for various trace-based security definitions [10,23,28]. Unlike our algorithms, these techniques focus on specific information-flow policies, not on a general logic like HyperLTL.

The use of prophecy variables [1] to make information about the future accessible is a known technique in the verification of trace properties. It is, for example, used to establish simulation relations between automata [26] or in the verification of CTL* properties [8].

In our game-theoretic view on the model checking problem for $\forall^*\exists^*$ hyperproperties the $\exists$-player has an infinite lookahead. There is some work on *finite* lookahead on trace languages [24]. We use the idea of finite lookahead as an approximation to construct existential strategies and give a novel synthesis construction for strategies with delay based on bounded synthesis [20].

2 Preliminaries

For tuples $\boldsymbol{x} \in X^n$ and $\boldsymbol{y} \in X^m$ over set X, we use $\boldsymbol{x} \cdot \boldsymbol{y} \in X^{n+m}$ to denote the concatenation of $\boldsymbol{x}$ and $\boldsymbol{y}$. Given a function $f\colon X \to Y$ and a tuple $\boldsymbol{x} \in X^n$, we define by $f \circ \boldsymbol{x} \in Y^n$ the tuple $(f(\boldsymbol{x}[1]), \dots, f(\boldsymbol{x}[n]))$. Let AP be a finite set of atomic propositions and let $\Sigma = 2^{\text{AP}}$ be the corresponding alphabet. A *trace* $t \in \Sigma^\omega$ is an infinite sequence of elements of Σ. We denote a set of traces by $Tr \subseteq \Sigma^\omega$. We define $t[i, \infty]$ to be the suffix of t starting at position $i \geq 0$.

HyperLTL. HyperLTL [6] is a temporal logic for specifying hyperproperties. It extends LTL by quantification over trace variables π and a method to link atomic propositions to specific traces. Let $\mathcal{V}$ be an infinite set of trace variables. Formulas in HyperLTL are given by the grammar

$$\varphi ::= \forall \pi.\, \varphi \mid \exists \pi.\, \varphi \mid \psi \ , \text{ and}$$
$$\psi ::= a_\pi \mid \neg\psi \mid \psi \vee \psi \mid \bigcirc \psi \mid \psi \,\mathcal{U}\, \psi \ ,$$

where $a \in \mathrm{AP}$ and $\pi \in \mathcal{V}$. We allow the standard boolean connectives $\wedge$, $\rightarrow$, $\leftrightarrow$ as well as the derived LTL operators release $\varphi \mathcal{R} \psi \equiv \neg(\neg\varphi \mathcal{U} \neg\psi)$, eventually $\Diamond\varphi \equiv \mathit{true}\ \mathcal{U}\ \varphi$, globally $\Box\varphi \equiv \neg\Diamond\neg\varphi$, and weak until $\varphi \mathcal{W} \psi \equiv \Box\varphi \vee (\varphi\ \mathcal{U}\ \psi)$.

We call a $\mathcal{Q}^+\mathcal{Q}'^+\varphi$ HyperLTL formula (for $\mathcal{Q}, \mathcal{Q}' \in \{\forall, \exists\}$ and quantifier-free formula φ) *alternation-free* iff $\mathcal{Q} = \mathcal{Q}'$. Further, we say that $\mathcal{Q}^+\mathcal{Q}'^+\varphi$ has *one quantifier alternation* (or lies in the *one-alternation fragment*) iff $\mathcal{Q} \neq \mathcal{Q}'$.

The semantics of HyperLTL is given by the satisfaction relation $\vDash_{Tr}$ over a set of traces $Tr \subseteq \Sigma^\omega$. We define an assignment $\Pi : \mathcal{V} \to \Sigma^\omega$ that maps trace variables to traces. $\Pi[\pi \mapsto t]$ updates Π by assigning variable π to trace t.

$$
\begin{array}{ll}
\Pi, i \vDash_{Tr} a_\pi & \text{iff } a \in \Pi(\pi)[i] \\
\Pi, i \vDash_{Tr} \neg\varphi & \text{iff } \Pi, i \nvDash_{Tr} \varphi \\
\Pi, i \vDash_{Tr} \varphi \vee \psi & \text{iff } \Pi, i \vDash_{Tr} \varphi \text{ or } \Pi, i \vDash_{Tr} \psi \\
\Pi, i \vDash_{Tr} \bigcirc\varphi & \text{iff } \Pi, i+1 \vDash_{Tr} \varphi \\
\Pi, i \vDash_{Tr} \varphi\,\mathcal{U}\,\psi & \text{iff } \exists j \geq i.\, \Pi, j \vDash_{Tr} \psi \wedge \forall i \leq k < j.\, \Pi, k \vDash_{Tr} \varphi \\
\Pi, i \vDash_{Tr} \exists\pi.\,\varphi & \text{iff there is some } t \in Tr \text{ such that } \Pi[\pi \mapsto t], i \vDash_{Tr} \varphi \\
\Pi, i \vDash_{Tr} \forall\pi.\,\varphi & \text{iff for all } t \in Tr \text{ it holds that } \Pi[\pi \mapsto t], i \vDash_{Tr} \varphi
\end{array}
$$

We write $Tr \vDash \varphi$ for $\{\}, 0 \vDash_{Tr} \varphi$ where $\{\}$ denotes the empty assignment.

Every hyperproperty is an intersection of a hypersafety and a hyperliveness property [7]. A *hypersafety* property is one where there is a finite set of finite traces that is a bad prefix, i.e., that cannot be extended into a set of traces that satisfies the hypersafety property. A *hyperliveness* property is a property where every finite set of finite traces can be extended to a possibly infinite set of infinite traces such that the resulting trace set satisfies the hyperliveness property.

Transition Systems. We use transition systems as a model of computation for reactive systems. Transition systems consume sequences over an input alphabet by transforming their internal state in every step. Let I and O be a finite set of input and output propositions, respectively, and let $\Upsilon = 2^I$ and $\Gamma = 2^O$ be the corresponding finite alphabets. A Γ-labeled Υ-*transition system* $\mathcal{S}$ is a tuple $\langle S, s_0, \tau, l\rangle$, where S is a finite set of states, $s_0 \in S$ is the designated initial state, $\tau\colon S \times \Upsilon \to S$ is the transition function, and $l\colon S \to \Gamma$ is the state-labeling function. We write $s \xrightarrow{\upsilon} s'$ or $(s, \upsilon, s') \in \tau$ if $\tau(s, \upsilon) = s'$. We generalize the transition function to sequences over Υ by defining $\tau^*\colon \Upsilon^* \to S$ recursively as $\tau^*(\epsilon) = s_0$ and $\tau^*(\upsilon_0 \cdots \upsilon_{n-1}\upsilon_n) = \tau(\tau^*(\upsilon_0 \cdots \upsilon_{n-1}), \upsilon_n)$ for $\upsilon_0 \cdots \upsilon_{n-1}\upsilon_n \in \Upsilon^+$. Given an infinite word $\upsilon = \upsilon_0\upsilon_1 \ldots \in \Upsilon^\omega$, the transition system produces an infinite sequence of outputs $\gamma = \gamma_0\gamma_1\gamma_2 \ldots \in \Gamma^\omega$, such that $\gamma_i = l(\tau^*(\upsilon_0 \ldots \upsilon_{i-1}))$ for every $i \geq 0$. The resulting *trace* ρ is $(\upsilon_0 \cup \gamma_0)(\upsilon_1 \cup \gamma_1) \ldots \in \Sigma^\omega$ where we have $AP = I \cup O$. The set of traces generated by $\mathcal{S}$ is denoted by $\mathit{traces}(\mathcal{S})$. Furthermore, we define $\varepsilon = \langle\{s\}, s, \tau_\varepsilon, l_\varepsilon\rangle$ as the transition system over $I = O = \emptyset$ that has only a single trace, that is $\mathit{traces}(\varepsilon) = \{\emptyset^\omega\}$. For this transition system, $\tau_\varepsilon(s, \emptyset) = s$ and $l_\varepsilon(s) = \emptyset$. Given two transition systems $\mathcal{S} = \langle S, s_0, \tau, l\rangle$ and $\mathcal{S}' = \langle S', s_0', \tau', l'\rangle$, we define $\mathcal{S} \times \mathcal{S}' = \langle S \times S', (s_0, s_0'), \tau'', l''\rangle$ as the Γ^2-labeled Υ^2-transition system where $\tau''((s, s'), (\upsilon, \upsilon')) = (\tau(s, \upsilon), \tau'(s', \upsilon'))$ and $l''((s, s')) = (l(s), l'(s'))$. A transition system $\mathcal{S}$ satisfies a general HyperLTL formula φ, if, and only if, $\mathit{traces}(\mathcal{S}) \vDash \varphi$.

Automata. An alternating parity automaton $\mathcal{A}$ over a finite alphabet Σ is a tuple $\langle Q, q_0, \delta, \alpha \rangle$, where Q is a finite set of states, $q_0 \in Q$ is the designated initial state, $\delta \colon Q \times \Sigma \to \mathbb{B}^+(Q)$ is the transition function, and $\alpha \colon Q \to C$ is a function that maps states of $\mathcal{A}$ to a finite set of colors $C \subset \mathbb{N}$. For $C = \{0, 1\}$ and $C = \{1, 2\}$, we call $\mathcal{A}$ a co-Büchi and Büchi automaton, respectively, and we use the sets $F \subseteq Q$ and $B \subseteq Q$ to represent the rejecting ($C = 1$) and accepting ($C = 2$) states in the respective automaton (as a replacement of the coloring function α). A safety automaton is a Büchi automaton where every state is accepting. The transition function δ maps a state $q \in Q$ and some $a \in \Sigma$ to a positive Boolean combination of successor states $\delta(q, a)$. An automaton is *non-deterministic* or *universal* if δ is purely disjunctive or conjunctive, respectively.

A run of an alternating automaton is a Q-labeled tree. A tree T is a subset of $\mathbb{N}_{>0}^*$ such that for every node $n \in \mathbb{N}_{>0}^*$ and every positive integer $i \in \mathbb{N}_{>0}$, if $n \cdot i \in T$ then (i) $n \in T$ (i.e., T is prefix-closed), and (ii) for every $0 < j < i$, $n \cdot j \in T$. The root of T is the empty sequence ϵ and for a node $n \in T$, $|n|$ is the length of the sequence n, in other words, its distance from the root. A run of $\mathcal{A}$ on an infinite word $\rho \in \Sigma^\omega$ is a Q-labeled tree (T, r) such that $r(\epsilon) = q_0$ and for every node $n \in T$ with children $n_1, \ldots, n_k$ the following holds: $1 \leq k \leq |Q|$ and $\{r(n_1), \ldots, r(n_k)\} \models \delta(q, \rho[i])$, where $q = r(n)$ and $i = |n|$. A path is accepting if the highest color appearing infinitely often is even. A run is accepting if all its paths are accepting. The language of $\mathcal{A}$, written $\mathcal{L}(\mathcal{A})$, is the set $\{\rho \in \Sigma^\omega \mid \mathcal{A} \text{ accepts } \rho\}$. A transition system $\mathcal{S}$ is accepted by an automaton $\mathcal{A}$, written $\mathcal{S} \models \mathcal{A}$, if $\mathit{traces}(\mathcal{S}) \subseteq \mathcal{L}(\mathcal{A})$.

Strategies. Given two disjoint finite alphabets Υ and Γ, a strategy $\sigma \colon \Upsilon^* \to \Gamma$ is a mapping from finite histories of Υ to Γ. A transition system $\mathcal{S} = \langle S, s_0, \tau, l \rangle$ *generates* the strategy σ if $\sigma(\boldsymbol{v}) = l(\tau^*(\boldsymbol{v}))$ for every $\boldsymbol{v} \in \Upsilon^*$. A strategy σ is called *finite-state* if there exists a transition system that generates σ.

In the following, we use finite-state strategies to modify the inputs of transition systems. Let $\mathcal{S} = \langle S, s_0, \tau, l \rangle$ be a transition system over input and output alphabets Υ and Γ and let $\sigma \colon (\Upsilon')^* \to \Upsilon$ be a finite-state strategy. Let $\mathcal{S}' = \langle S', s_0', \tau', l' \rangle$ be the transition system implementing σ, then $\mathcal{S} \,||\, \sigma = \mathcal{S} \,||\, \mathcal{S}'$ is the transition system $\langle S \times S', (s_0, s_0'), \tau^{||}, l^{||} \rangle$ where $\tau^{||} \colon (S \times S') \times \Upsilon' \to (S \times S')$ is defined as $\tau^{||}((s, s'), \upsilon') = (\tau(s, l'(s')), \tau'(s', \upsilon'))$ and $l^{||} \colon (S \times S') \to \Gamma$ is defined as $l^{||}(s, s') = l(s)$ for every $s \in S$, $s' \in S'$, and $\upsilon' \in \Upsilon'$.

Model Checking HyperLTL. We recap the model checking of universal HyperLTL formulas. This case, as well as the dual case of only existential quantifiers, is well-understood and, in fact, efficiently implemented in the model checker MCHyper [18]. The principle behind the model checking approach is *self-composition*, where we check a standard trace property on a composition of an appropriate number of copies of the given system.

Let *zip* denote the function that maps an n-tuple of sequences to a single sequence of n-tuples, for example, $\mathit{zip}([1, 2, 3], [4, 5, 6]) = [(1, 4), (2, 5), (3, 6)]$, and let *unzip* denote its inverse. Given $\mathcal{S} = \langle S, s_0, \tau, l \rangle$, the n-fold self-composition of $\mathcal{S}$ is the transition system $\mathcal{S}^n = \langle S^n, \boldsymbol{s_0'}, \tau_n, l_n \rangle$, where $\boldsymbol{s_0'} \coloneqq (s_0, \ldots, s_0) \in S^n$, $\tau_n(\boldsymbol{s}, \boldsymbol{v}) \coloneqq \tau \circ \mathit{zip}(\boldsymbol{s}, \boldsymbol{v})$ and $l_n(\boldsymbol{s}) \coloneqq l \circ \boldsymbol{s}$ for every $\boldsymbol{s} \in S^n$ and $\boldsymbol{v} \in \Upsilon^n$. If $\mathit{traces}(\mathcal{S})$

is the set of traces generated by $\mathcal{S}$, then $\{zip(\rho_1, \ldots, \rho_n) \mid \rho_1, \ldots, \rho_n \in traces(\mathcal{S})\}$ is the set of traces generated by $\mathcal{S}^n$. We use the notation $zip(\varphi, \pi_1, \pi_2, \ldots, \pi_n)$ for some HyperLTL formula φ to combine the trace variables $\pi_1, \pi_2, \ldots, \pi_n$ (occurring free in φ) into a fresh trace variable π^*.

Theorem 1 (Self-composition for universal HyperLTL formulas [18]). *For a transition system $\mathcal{S}$ and a HyperLTL formula of the form $\forall \pi_1. \forall \pi_2. \ldots \forall \pi_n.\ \varphi$ it holds that $\mathcal{S} \vDash \forall \pi_1. \forall \pi_2. \ldots \forall \pi_n.\ \varphi$ iff $\mathcal{S}^n \vDash \forall \pi^*.\ zip(\varphi, \pi_1, \pi_2, \ldots, \pi_n)$.*

Theorem 2 (Complexity of model checking universal formulas [18]). *The model checking problem for universal HyperLTL formulas is PSPACE-complete in the size of the formula and NLOGSPACE-complete in the size of the transition system.*

The complexity of verifying universal HyperLTL formulas is exactly the same as the complexity of verifying LTL formulas. For HyperLTL formulas with quantifier alternations, the model checking problem is significantly more difficult.

Theorem 3 (Complexity of model checking formulas with one quantifier alternation [18]). *The model checking problem for HyperLTL formulas with one quantifier alternation is in EXPSPACE in the size of the formula and in PSPACE in the size of the transition system.*

One way to circumvent this complexity is to fix the existential choice and strengthen the formula to the universal fragment [9,13,18]. While avoiding the complexity problem, this transformation requires deep knowledge of the system, is prone to errors, and cannot be verified automatically as the problem of checking implications becomes undecidable [11]. In the following section, we present a technique that circumvents the complexity problem while still inheriting strong correctness guarantees. Further, we provide a method that can, under certain restrictions, derive a strategy for the existential choice automatically.

3 Model Checking with Quantifier Alternations

3.1 Model Checking with Given Strategies

Our first goal is the verification of HyperLTL formulas with one quantifier alternation, i.e., formulas of the form $\forall^* \exists^* \varphi$ or $\exists^* \forall^* \varphi$, where φ is a quantifier-free formula. Note that the presented techniques can, similar to skolemization, be extended to more than one quantifier alternation. Quantifier alternation introduces dependencies between the quantified traces. In a $\forall^* \exists^* \varphi$ formula, the choices of the existential quantifiers depend on the choices of the universal quantifiers preceding them. In a formula of the form $\exists^* \forall^* \varphi$, however, there has to be a single choice for the existential quantifiers that works for all choices of the universal quantifiers. In this case, the existentially quantified variables do not depend on the universally quantified variables. Hence, the witnesses for the existential quantifiers are traces rather than functions that map tuples of traces

to traces. As established above, the model checking problem for HyperLTL formulas with quantifier alternation is known to be significantly more difficult than the model checking problem for universal formulas.

Our verification technique for formulas with quantifier alternation is to substitute strategic choice for existential choice. As discussed in the introduction, the existence of a strategy implies the existence of a trace.

Theorem 4 (Substituting Strategic Choice for Existential Choice). *Let $\mathcal{S}$ be a transition system over input alphabet Υ.*
It holds that $\mathcal{S} \vDash \forall\pi_1\forall\pi_2 \dots \forall\pi_n.\ \exists\pi'_1\exists\pi'_2 \dots \exists\pi'_m.\ \varphi$ if there is a strategy $\sigma : (\Upsilon^n)^* \to \Upsilon^m$ such that $\mathcal{S}^n \times (\mathcal{S}^m \mid\mid \sigma) \vDash \forall\pi^*.zip(\varphi, \pi_1, \pi_2, \dots \pi_n, \pi'_1, \pi'_2, \dots, \pi'_m)$.
It holds that $\mathcal{S} \vDash \exists\pi_1\exists\pi_2 \dots \exists\pi_m.\ \forall\pi'_1\forall\pi'_2 \dots \forall\pi'_n.\ \varphi$ if there is a strategy $\sigma : (\Upsilon^0)^* \to \Upsilon^m$ such that $(\mathcal{S}^m \mid\mid \sigma) \times \mathcal{S}^n \vDash \forall\pi^*.zip(\varphi, \pi_1, \pi_2, \dots \pi_m, \pi'_1, \pi'_2, \dots, \pi'_n)$.

Proof. Let σ be such a strategy, then we define a witness for the existential trace quantifiers $\exists\pi'_1\exists\pi'_2 \dots \exists\pi'_m$ as the sequence of inputs $\upsilon = \upsilon_0\upsilon_1 \dots \in (\Upsilon^m)^\omega$ such that $\upsilon_i = \sigma(\upsilon'_0\upsilon'_1 \dots \upsilon'_{i-1})$ for every $i \geq 0$ and every $\upsilon'_i \in \Upsilon^n$; analogously, we define a witness for the existential trace quantifiers $\exists\pi_1\exists\pi_2 \dots \exists\pi_m$ as the sequence of inputs $\upsilon = \upsilon_0\upsilon_1 \dots \in (\Upsilon^m)^\omega$ such that $\upsilon_i = \sigma(\upsilon'_0\upsilon'_1 \dots \upsilon'_{i-1})$ for every $i \geq 0$ and every $\upsilon'_i \in \Upsilon^0$. □

An application of the theorem reduces the verification problem of a HyperLTL formula with one quantifier alternation to the verification problem of a universal HyperLTL formula. If a sufficiently small strategy can be found, the reduction in complexity is substantial:

Corollary 1 (Model checking with Given Strategies). *The model checking problem for HyperLTL formulas with one quantifier alternation and given strategies for the existential quantifiers is in PSPACE in the size of the formula and NLOGSPACE in the size of the product of the strategy and the system.*

Note that the converse of Theorem 4 is not in general true. The satisfaction of a $\forall^*\exists^*$ HyperLTL formula does not imply the existence of a strategy, because at any given point in time the strategy only knows about a finite prefix of the universally quantified traces. Consider the formula $\forall\pi\exists\pi'.\bigcirc a_\pi \leftrightarrow a_{\pi'}$ and a system that can produce arbitrary sequences of a and $\neg a$. Although the system satisfies the formula, it is not possible to give a strategy that allows us to prove this fact. Whatever choice our strategy makes, the next move of the $\forall$-player can make sure that the strategy's choice was wrong. In the following, we present a method that addresses this problem.

Prophecy Variables. A classic technique for resolving future dependencies is the introduction of *prophecy variables* [1]. Prophecy variables are auxiliary variables that are added to the system without affecting the behavior of the system. Such variables can be used to make predictions about the future.

We use prophecy variables to define strategies that depend on the future. In the example discussed above, $\forall\pi\exists\pi'.\bigcirc a_\pi \leftrightarrow a_{\pi'}$, the choice of the value of $a_{\pi'}$ in

the first position depends on the value of a_π in the second position. We introduce a prophecy variable p that predicts in the first position whether a_π is true in the second position. With the prophecy variable, there exists a strategy that correctly assigns the value of p whenever the prediction is correct: The strategy chooses to set $a_{\pi'}$ if, and only if, p holds.

Technically, the proof technique introduces a set of fresh input variables P into the system. For a Γ-labeled Υ-transition system $\mathcal{S} = \langle S, s_0, \tau, l\rangle$, we define the Γ-labeled $(\Upsilon \cup P)$-transition system $\mathcal{S}^P = \langle S, s_0, \tau^P, l\rangle$ including the inputs P where $\tau^P \colon S \times (\Upsilon \cup P) \to S$. For all $s \in S$ and $\upsilon^P \in \Upsilon \cup P$, $\tau^P(s, \upsilon^P) = \tau(s, \upsilon)$ for $\upsilon \in \Upsilon$ obtained by removing the variables in P from υ^P (i.e., $\upsilon =_{\setminus P} \upsilon^P$). Moreover, the proof technique modifies the specification so that the original property only needs to be satisfied if the prediction is actually correct. We obtain the modified specification $\forall\pi\exists\pi'.(p_\pi \leftrightarrow \bigcirc a_\pi) \rightarrow (\bigcirc a_\pi \leftrightarrow a_{\pi'})$ in our example. The following theorem describes the general technique for one prophecy variable.

Theorem 5 (Model checking with Prophecy Variables). *For a transition system $\mathcal{S}$ and a quantifier-free formula φ, let ψ be a quantifier-free formula over the universally quantified trace variables $\pi_1, \pi_2 \dots \pi_n$ and let p be a fresh atomic proposition. It holds that $\mathcal{S} \vDash \forall\pi_1\forall\pi_2 \dots \forall\pi_n.\ \exists\pi'_1\exists\pi'_2 \dots \exists\pi'_m.\ \varphi$ if, and only if, $\mathcal{S}^{\{p\}} \vDash \forall\pi_1\forall\pi_2 \dots \forall\pi_n.\ \exists\pi'_1\exists\pi'_2 \dots \exists\pi'_m.\square(p_{\pi_1} \leftrightarrow \psi) \rightarrow \varphi$.*

Note that ψ is restricted to refer only to *universally* quantified trace variables. Without this restriction, the method would not be sound. In our example, $\psi = a_{\pi'}$ would lead to the modified formula $\forall\pi\exists\pi'.(p_\pi \leftrightarrow a_{\pi'}) \rightarrow (\bigcirc a_\pi \leftrightarrow a_{\pi'})$, which could be satisfied with the strategy that assigns $a_{\pi'}$ to *true* iff p_π is *false*, and thus falsifies the assumption that the prediction is correct, rather than ensuring that the original formula is true.

Proof. It is easy to see that the original specification implies the modified specification, since the original formula is the conclusion of the implication. Assume that the modified specification holds. Since the prophecy variable p is a fresh atomic proposition, and ψ does not refer to the existentially chosen traces, we can, for every choice of the universally quantified traces, always choose the value of p such that it guesses correctly, i.e., that p is true whenever ψ holds. In this case, the conclusion and therefore the original specification must be true. □

Unfortunately, prophecy variables do not provide a complete proof technique. Consider a system allowing arbitrary sequences of a and b and this specification:

$$\begin{aligned}\forall\pi\exists\pi'.b_{\pi'} \wedge \square(b_{\pi'} \leftrightarrow \bigcirc \neg b_{\pi'})\\ \wedge (a_{\pi'} \rightarrow (a_\pi \mathcal{W} (b_{\pi'} \wedge \neg a_\pi)))\\ \wedge (\neg a_{\pi'} \rightarrow (a_\pi \mathcal{W} (\neg b_{\pi'} \wedge \neg a_\pi)))\end{aligned}$$

Intuitively, π' has to be able to predict whether π will stop outputting a at an even or odd position of the trace. There is no HyperLTL formula to be used as ψ in Theorem 5, because, like LTL, HyperLTL can only express non-counting properties. It is worth noting that in our practical experiments, the

incompleteness was never a problem. In many cases, it is not even necessary to add prophecy variables at all. The presented proof technique is, thus, practically useful despite this incompleteness result.

3.2 Model Checking with Synthesized Strategies

We now extend the model checking approach with the automatic synthesis of the strategies for the existential quantifiers. For a given HyperLTL formula of the form $\forall^n \exists^m \varphi$ and a transition system $\mathcal{S}$, we search for a transition system $\mathcal{S}_\exists = \langle X, x_0, \mu, l_\exists \rangle$, where X is a set of states, $x_0 \in X$ is the designated initial state, $\mu \colon X \times \Upsilon^n \to X$ is the transition function, and $l_\exists \colon X \to \Upsilon^m$ is the labeling function, such that $\mathcal{S}^n \times (\mathcal{S}^m \mid\mid \mathcal{S}_\exists) \vDash \mathit{zip}(\varphi)$. (Since for formulas of the form $\exists^m \forall^n \varphi$ the problem only differs in the input of $\mathcal{S}_\exists$, we focus on $\forall\exists$ HyperLTL.)

Theorem 6. *The strategy realizability problem for $\forall^*\exists^*$ formulas is* 2ExpTime*-complete.*

Proof (Sketch). We reduce the strategy synthesis problem to the problem of synthesizing a distributed reactive system with a single black-box process. This problem is decidable [19] and can be solved in 2ExpTime. The lower bound follows from the LTL realizability problem [30]. □

The decidability result implies that there is an upper bound on the size of $\mathcal{S}_\exists$ that is doubly exponential in φ. Thus, the bounded synthesis approach [20] can be used to search for increasingly larger implementations, until a solution is found or the maximal bound is reached, yielding an efficient decision procedure for the strategy synthesis problem. In the following, we describe this approach in detail.

Bounded Synthesis of Strategies. We transform the synthesis problem into an SMT constraint satisfaction problem, where we leave the representation of strategies uninterpreted and challenge the solver to provide an interpretation. Given a HyperLTL formula $\forall^n \exists^m \varphi$ where φ is quantifier-free, the model checking is based on the product of the n-fold self composition of the transition system $\mathcal{S}$, the m-fold self-composition of $\mathcal{S}$ where the strategy $\mathcal{S}_\exists$ controls the inputs, and the universal co-Büchi automaton $\mathcal{A}_\varphi$ representing the language $\mathcal{L}(\varphi)$ of φ.

For a quantifier-free HyperLTL formula φ, we construct the universal co-Büchi automaton $\mathcal{A}_\varphi$ such that $\mathcal{L}(\mathcal{A}_\varphi)$ is the set of words w such that $\mathit{unzip}(w) \vDash \varphi$, i.e., the tuple of traces satisfies φ. We get this automaton by dualizing the non-deterministic Büchi automaton for $\neg\psi$ [6], i.e., changing the branching from non-deterministic to universal and the acceptance condition from Büchi to co-Büchi. Hence, $\mathcal{S}$ satisfies a universal HyperLTL formula $\forall \pi_1 \ldots \forall \pi_n . \varphi$ if the traces generated by the self-composition $\mathcal{S}^n$ are a subset of $\mathcal{L}(\mathcal{A}_\varphi)$.

In more detail, the algorithm searches for a transition system $\mathcal{S}_\exists = \langle X, x_0, \mu, l_\exists \rangle$ such that the run graph of $\mathcal{S}^n$, $\mathcal{S}^m \mid\mid \mathcal{S}_\exists$, and $\mathcal{A}_\varphi$, written $\mathcal{S}^n \times (\mathcal{S}^m \mid\mid \mathcal{S}_\exists) \times \mathcal{A}_\varphi$, is accepting. Formally, given a Γ-labeled Υ-transition

system $\mathcal{S} = \langle S, s_0, \tau, l\rangle$ and a universal co-Büchi automaton $\mathcal{A}_\varphi = \langle Q, q_0, \delta, F\rangle$, where $\delta\colon Q \times \Upsilon^{n+m} \times \Gamma^{n+m} \to 2^Q$, the run graph $\mathcal{S}^n \times (\mathcal{S}^m \mid\mid \mathcal{S}_\exists) \times \mathcal{A}_\varphi$ is the directed graph (V, E), with the set of vertices $V = S^n \times S^m \times X \times Q$, initial vertex $v_{init} = ((s_0, \dots, s_0), (s_0, \dots, s_0), x_0, q_0)$ and the edge relation $E \subseteq V \times V$ satisfying $((\boldsymbol{s_n}, \boldsymbol{s_m}, x, q), (\boldsymbol{s'_n}, \boldsymbol{s'_m}, x', q')) \in E$ if, and only if

$$\exists \boldsymbol{\upsilon} \in \Upsilon^n.\ \left(\boldsymbol{s_n} \xrightarrow[\tau_n]{\upsilon} \boldsymbol{s'_n}\right) \wedge \left(\boldsymbol{s_m} \xrightarrow[\tau_m]{l_\exists(x)} \boldsymbol{s'_m}\right) \wedge \left(x \xrightarrow[\mu]{\upsilon} x'\right) \wedge q' \in \delta(q, \boldsymbol{\upsilon} \cdot l_\exists(x), l_n(\boldsymbol{s_n}) \cdot l_m(\boldsymbol{s_m})).$$

Theorem 7. *Given $\mathcal{S}$, $\mathcal{S}_\exists$, and a HyperLTL formula $\forall^n \exists^m \varphi$ where φ is quantifier-free. Let $\mathcal{A}_\varphi$ be the universal co-Büchi automaton for φ. If the run graph $\mathcal{S}^n \times (\mathcal{S}^m \mid\mid \mathcal{S}_\exists) \times \mathcal{A}_\varphi$ is accepting, then $\mathcal{S} \vDash \forall^n \exists^m \varphi$.*

Proof. Follows from Theorem 4 and the fact that $\mathcal{A}_\varphi$ represents $\mathcal{L}(\varphi)$. □

The acceptance of a run graph is witnessed by an annotation $\lambda\colon V \to \mathbb{N} \cup \{\bot\}$ which is a function mapping every reachable vertex $v \in V$ in the run graph to a natural number $\lambda(v)$, i.e., $\lambda(v) \neq \bot$. Intuitively, $\lambda(v)$ returns the number of visits to rejecting states on any path from the initial vertex v_{init} to v. If we can bound this number for every reachable vertex, the annotation is *valid* and the run graph is accepting. Formally, an annotation λ is valid, if (1) the initial state is reachable ($\lambda(v_{init}) \neq \bot$) and (2) for every $(v, v') \in E$ with $\lambda(v) \neq \bot$ it holds that $\lambda(v') \neq \bot$ and $\lambda(v) \rhd \lambda(v')$ where $\trianglerighteq$ is $>$ if v' is rejecting and $\geq$ otherwise. Such an annotation exists if, and only if, the run graph is accepting [20].

We encode the search for $\mathcal{S}_\exists$ and the annotation λ as an SMT constraint system. Therefore, we use uninterpreted function symbols to encode $\mathcal{S}_\exists$ and λ. A transition system $\mathcal{S}$ is represented in the constraint system by two functions, the transition function $\tau\colon S \times \Upsilon \to S$ and the labeling function $l\colon S \to \Gamma$. The annotation is split into two parts, a reachability constraint $\lambda^{\mathbb{B}}\colon V \to \mathbb{B}$ indicating whether a state in the run graph is reachable and a counter $\lambda^{\#}\colon V \to \mathbb{N}$ that maps every reachable vertex v to the maximal number of rejecting states $\lambda^{\#}(v)$ visited by any path from the initial vertex to v. The resulting constraint asserts that there is a transition system $\mathcal{S}_\exists$ with an accepting run graph. Note, that the functions representing the system $\mathcal{S}$ ($\tau\colon S \times \Upsilon \to S$ and $l\colon S \to \Gamma$) are given, that is, they are interpreted.

$$\begin{aligned}
&\exists \lambda^{\mathbb{B}}\colon S^n \times S^m \times X \times Q \to \mathbb{B}.\ \exists \lambda^{\mathbb{N}}\colon S^n \times S^m \times X \times Q \to \mathbb{N}.\\
&\exists \mu\colon X \times \Upsilon^n \to X.\ \exists l_\exists\colon X \to \Upsilon^m\\
&\forall \boldsymbol{\upsilon} \in \Upsilon^n.\ \forall \boldsymbol{s_n}, \boldsymbol{s'_n} \in S^n.\ \forall \boldsymbol{s_m}, \boldsymbol{s'_m} \in S^m.\ \forall q, q' \in Q.\ \forall x, x' \in X.\\
&\lambda^{\mathbb{B}}((s_0, \dots, s_0), (s_0, \dots, s_0), x_0, q_0) \wedge\\
&\Big(\lambda^{\mathbb{B}}(\boldsymbol{s_n}, \boldsymbol{s_m}, x, q) \wedge q' \in \delta(q, (\boldsymbol{\upsilon} \cdot l_\exists(x)), (l \circ (\boldsymbol{s_n} \cdot \boldsymbol{s_m}))) \wedge x' = \mu(x, \boldsymbol{\upsilon})\\
&\quad \wedge \boldsymbol{s'_n} = \tau_n(\boldsymbol{s_n}, \boldsymbol{\upsilon}) \wedge \boldsymbol{s'_m} = \tau_m(\boldsymbol{s_m}, l_\exists(x))\Big)\\
&\Rightarrow \lambda^{\mathbb{B}}(\boldsymbol{s'_n}, \boldsymbol{s'_m}, x', q') \wedge \lambda^{\mathbb{N}}(\boldsymbol{s_n}, \boldsymbol{s_m}, x, q) \trianglerighteq \lambda^{\mathbb{N}}(\boldsymbol{s'_n}, \boldsymbol{s'_m}, x', q')
\end{aligned}$$

where $\trianglerighteq$ is $>$ if $q' \in F$ and $\geq$ otherwise. The *bounded synthesis algorithm* increases the bound of the strategy $\mathcal{S}_\exists$ until either the constraints system becomes satisfiable, or a given upper bound is reached. In the case the constraint system is satisfiable, we can extract interpretations for the functions μ and $l_\exists$ using a solver that is able to produce models. These functions then represent the synthesized transition system $\mathcal{S}_\exists$.

Corollary 2. *Given $\mathcal{S}$ and a HyperLTL formula $\forall^*\exists^*\varphi$ where φ is quantifier-free. If the constraint system is satisfiable for some bound on the size of $\mathcal{S}_\exists$ then $\mathcal{S} \vDash \forall^*\exists^*\varphi$.*

Proof. Follows immediately by Theorem 7. □

As the decision problem is decidable, we know that there is an upper bound on the size of a realizing $\mathcal{S}_\exists$ and, thus, the bounded synthesis approach is a decision procedure for the strategy realizability problem.

Corollary 3. *The bounded synthesis algorithm decides the strategy realizability problem for $\forall^*\exists^*$ HyperLTL.*

Proof. The existence of such an upper bound follows from Theorem 6. □

Approximating Prophecy. We introduce a new parameter to the strategy synthesis problem to approximate the information about the future that can be captured using prophecy variables. This bound represents a constant *lookahead* into future choices made by the environment. In other words, for a given $k \geq 0$, the strategy $\mathcal{S}_\exists$ is allowed to depend on choices of the $\forall$-player in the next k steps. While constant lookahead is only an approximation of infinite clairvoyance, it suffices for many practical situations as shown by prior case studies [9,18].

We present a solution to synthesizing transition systems with constant lookahead for $k \geq 0$ using bounded synthesis. To simplify the presentation, we present the stand-alone problem with respect to a specification given as a universal co-Büchi automaton. The integration into the constraint system for the $\forall^*\exists^*$ HyperLTL synthesis as presented in the previous section is then straightforward. First, we present an extension to the transition system model that incorporates the notion of constant lookahead. The idea of this extension is to replace the initial state s_0 by a function $init\colon \Upsilon^k \to S$ that maps input sequences of length k to some state. Thus, the transition system observes the first k inputs, chooses some initial state based on those inputs, and then progresses with the same pace as the input sequence. Next, we define the run graph of such a system $\mathcal{S}_k = \langle S, init, \tau, l\rangle$ and an automaton $\mathcal{A} = \langle Q, q_0, \delta, F\rangle$, where $\delta\colon Q \times \Upsilon \times \Gamma \to Q$, as the directed graph (V, E) with the set of vertices $V = S \times Q \times \Upsilon^k$, the initial vertices $(s, q_0, \boldsymbol{v}) \in V$ such that $s = init(\boldsymbol{v})$ for every $\boldsymbol{v} \in \Upsilon^k$, and the edge relation $E \subseteq V \times V$ satisfying $((s, q, v_1 v_2 \cdots v_k), (s', q', v_1' v_2' \cdots v_k')) \in E$ if, and only if

$$\exists v_{k+1} \in \Upsilon.\, s \xrightarrow{v_{k+1}} s' \wedge q' \in \delta(q, v_1, l(s)) \wedge \bigwedge_{1 \leq i \leq k} v_i' = v_{i+1}.$$

Lemma 1. *Given a universal co-Büchi automaton $\mathcal{A}$ and a k-lookahead transition system $\mathcal{S}_k$. $\mathcal{S}_k \vDash \mathcal{A}$ if, and only if, the run graph $\mathcal{S}_k \times \mathcal{A}$ is accepting.*

Finally, synthesis amounts to solving the following constraint system:

$$
\begin{aligned}
&\exists \lambda^{\mathbb{B}} \colon S \times Q \times \Upsilon^k \to \mathbb{B}.\, \exists \lambda^{\mathbb{N}} \colon S \times Q \times \Upsilon^k \to \mathbb{N}. \\
&\exists \mathit{init} \colon \Upsilon^k \to S.\, \exists \tau \colon S \times \Upsilon \to S.\, \exists l \colon S \to \Gamma. \\
&(\forall \boldsymbol{\upsilon} \in \Upsilon^k.\, \lambda^{\mathbb{B}}(\mathit{init}(\boldsymbol{\upsilon}), q_0, \boldsymbol{\upsilon})) \wedge \\
&\forall \upsilon_1 \upsilon_2 \cdots \upsilon_{k+1} \in \Upsilon^{k+1}.\, \forall s, s' \in S.\, \forall q, q' \in Q. \\
&\big(\lambda^{\mathbb{B}}(s, q, \upsilon_1 \cdots \upsilon_k) \wedge s' = \tau(s, \upsilon_{k+1}) \wedge q' \in \delta(q, \upsilon_1, l(s))\big) \\
&\Rightarrow \lambda^{\mathbb{B}}(s', q', \upsilon_2 \cdots \upsilon_{k+1}) \wedge \lambda^{\mathbb{N}}(s, q, \upsilon_1 \cdots \upsilon_k) \trianglerighteq \lambda^{\mathbb{N}}(s', q', \upsilon_2 \cdots \upsilon_{k+1})
\end{aligned}
$$

Corollary 4. *Given some $k \geq 0$, if the constraint system is satisfiable for some bound on the size of $\mathcal{S}_k$ then $\mathcal{S}_k \vDash \mathcal{A}$.*

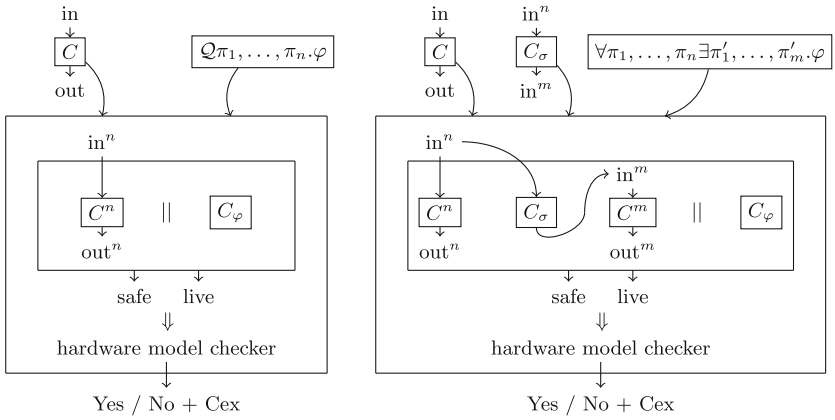
4 Synthesis with Quantifier Alternations

We now build on the introduced techniques to solve the *synthesis* problem for HyperLTL with quantifier alternation, that is, we search for implementations that satisfy the given properties. In previous work [13], the synthesis problem for $\exists^*\forall^*$ HyperLTL was solved by a reduction to the distributed synthesis problem. We present an alternative synthesis procedure that (1) introduces the necessary concepts for the synthesis of the $\forall^*\exists^*$ fragment and that (2) strictly decomposes the choice of the existential trace quantifier from the implementation.

Fix a formula of the form $\exists^m \forall^n \varphi$. We again reduce the verification problem to the problem of determining whether a run graph is accepting. As the existential quantifiers do not depend on the universal ones, there is no future dependency and thus no need for prophecy variables or bounded lookahead. Formally, $\mathcal{S}_\exists$ is a tuple $\langle X, x_0, \mu, l_\exists \rangle$ such that X is a set of states, $x_0 \in X$ is the designated initial state, $\mu \colon X \to X$ is the transition function, and $l_\exists \colon X \to \Upsilon^m$ is the labeling function. $\mathcal{S}_\exists$ produces infinite sequences of $(\Upsilon^m)^\omega$, without having any knowledge about the behavior of the universally quantified traces. The run graph is then $(\mathcal{S}^m \mid\mid \mathcal{S}_\exists) \times \mathcal{S}^n \times \mathcal{A}_\varphi$. The constraint system is built analogously to Sect. 3.2, with the difference that the representation of the system $\mathcal{S}$ is now also uninterpreted. In the resulting SMT constraint system, we have two bounds, one for the size of the implementation $\mathcal{S}$ and one for the size of $\mathcal{S}_\exists$.

Corollary 5. *The bounded synthesis algorithm decides the realizability problem for $\exists^*\forall^1$ HyperLTL and is a semi-decision procedure for $\exists^*\forall^{>1}$ HyperLTL.*

The synthesis problem for formulas in the $\forall^*\exists^*$ HyperLTL fragment uses the same reduction to a constraint system as the strategy synthesis in Sect. 3.2, with the only difference that the transition system $\mathcal{S}$ itself is uninterpreted. In the resulting SMT constraint systems, we have three bounds, the size of the implementation $\mathcal{S}$, the size of the strategy $\mathcal{S}_\exists$, and the lookahead k.



(a) Alternation-free model checking with self-composition

(b) One-alternation model checking with given strategy (case $\forall^n\exists^m$ HyperLTL)

Fig. 1. HyperLTL model checking with MCHyper

Corollary 6. *Given a HyperLTL formula $\forall^n\exists^m\varphi$ where φ is quantifier-free. $\forall^n\exists^m\varphi$ is realizable if the SMT constraint system corresponding to the run graph $\mathcal{S}^n \times (\mathcal{S}^m \mid\mid \mathcal{S}_\exists) \times \mathcal{A}_\varphi$ is satisfiable for some bounds on $\mathcal{S}$, $\mathcal{S}_\exists$, and lookahead k.*

5 Implementations and Experimental Evaluation

We have integrated the model checking technique with a manually provided strategy into the HyperLTL hardware model checker MCHyper[1]. For the synthesis of strategies and reactive systems from hyperproperties, we have developed a separate bounded synthesis tool based on SMT-solving. In the following, we describe these implementations and report on experimental results. All experiments ran on a machine with dual-core Core i7, 3.3 GHz, and 16 GB memory.

Hardware Model Checking with Given Strategies. We have extended the model checker MCHyper [18] from the alternation-free fragment to formulas with one quantifier alternation. The input to MCHyper is a circuit description as an And-Inverter-Graph in the Aiger format and a HyperLTL formula. Figures 1a and 1 show the model checking process in MCHyper without and with quantifier alternation, respectively. For formulas with quantifier alternation, the model checker now also accepts a strategy as an additional Aiger circuit C_σ. Based on this strategy, MCHyper creates a new circuit where only the inputs of the universal system copies are exposed and the inputs of the existential system

[1] Try the online tool interface with the latest version of MCHyper: https://www.react.uni-saarland.de/tools/online/MCHyper/.

Table 1. Experimental results for MCHyper on the software doping and mutual exclusion benchmarks. All experiments used the IC3 option for abc. Model and property names correspond to the ones used in [9] and [18].

Model	#Latches	Property	Time[s]
EC 0.05	17	$(10.a) + (10.b)$	1.8
EC 0.00625	23	$(10.a) + (10.b)$	53.4
AEC 0.05	19	$(\neg 10.a) + (\neg 10.b)$	2.8
AEC 0.00625	25	$(\neg 10.a) + (\neg 10.b)$	160.1
Bakery.a.n.s	47	Sym5	50.6
		Sym6	27.5
Bakery.a.n.s.5proc	90	Sym7	461.3
		Sym8	472.3

copies are determined by the strategy. The new circuit is then model checked as described in [18] with abc [4].

We evaluate our extension of MCHyper on formulas with quantifier alternation based on benchmarks from software doping [9] and symmetry in mutual exclusion algorithms [18]. Both considered problems have previously been analyzed with MCHyper; however, since the properties in both problems require quantifier alternation, we were previously limited to a (manually obtained) approximation of the properties as universal formulas. The correctness of manual approximations is not given but has to be shown separately. By directly model checking the formula with quantifier alternation we know that we are checking the correct formula without needing any additional proof of correctness.

Software Doping. D'Argenio et al. [9] examined a clean and a doped version of an emission control program of a car and used the previous version of MCHyper to formally verify approximations of these properties. Robust cleanness is expressed in the one-alternation fragment using two $\forall^2\exists^1$ HyperLTL formulas (given in Prop. 19 in [9], cf. Sect. 1). In [9], the formulas were strengthened into alternation-free formulas that imply the original properties. Despite the quantifier alternation, Table 1 shows that the new version of MCHyper verifies the precise formulas in roughly the same time as the alternation-free approximations [9] while giving stronger correctness guarantees.

Symmetry in Mutual Exclusion Protocols. $\forall^*\exists^*$ HyperLTL allows us to specify symmetry for mutual exclusion protocols. In such protocols, we wish to guarantee that every request is eventually answered, and the grants are mutually exclusive. In our experiments, we used an implementation of the Bakery protocol [25]. Table 1 shows the verification results for the precise $\forall^1\exists^1$ properties. Comparing these results to the performance on the approximations of the symmetry properties [18], we, again, observe that the verification times are similar. However, we gain the additional correctness guarantees as described above.

Strategy and System Synthesis. For the synthesis of strategies for existential quantifiers and for the synthesis of reactive systems from hyperproperties, we have developed a separate bounded synthesis tool based on SMT-solving with z3 [29]. Our evaluation is based on two benchmark families, the *dining cryptographers* problem [5] and a simplified version of the symmetry problem in mutual exclusion protocols discussed previously. The results are shown in Table 2. Obviously, synthesis operates at a vastly smaller scale than model checking with given strategies. In the dining cryptographers example, z3 was unable to find an implementation for the full synthesis problem, but could easily synthesize strategies for the existential trace quantifiers when provided with an implementation. With the progress of constraint solver that employ quantification over Boolean functions [31] we expect scalability improvements of our synthesis approach.

Table 2. Summary of the experimental results on the benchmarks sets described in Sect. 5. When no hyperproperty is given, only the LTL part is used.

Instance	Hyperproperty	$\lvert\mathcal{S}\rvert$	$\lvert\mathcal{S}_\exists\rvert$	Time [s]
Dining cryptographers	distributed + deniability			TO
	distributed + deniability with given $\mathcal{S}$	(1)	1	1.2
Mutex	—	2	–	<1
	symmetry	3	1	3.4
Mutex w/o spurious grants	—	3	–	<1
	symmetry	3	1	3.9
	wait-free	3	3	46
	symmetry + wait-free	3	1 + 3	840

6 Conclusions

We have presented model checking and synthesis techniques for hyperliveness properties expressed as HyperLTL formulas with quantifier alternation. The alternation makes it possible to specify hyperproperties such as generalized noninterference, symmetry, and deniability. Our approach is the first method for the synthesis of reactive systems from HyperLTL formulas with quantifier alternation and the first practical method for the verification of such specifications.

The approach is based on a game-theoretic view of existential quantifiers, where the $\exists$-player reacts to decisions of the $\forall$-player. The key advantage is that the complementation of the system automaton is avoided (cf. [18]). Instead, a strategy must be found for the $\exists$-player. Since this can be done either manually or through automatic synthesis, the user of the model checking or synthesis tool has the opportunity to trade some automation for a significant gain in performance.

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Quantitative Mitigation of Timing Side Channels

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Abstract. Timing side channels pose a significant threat to the security and privacy of software applications. We propose an approach for *mitigating* this problem by decreasing the strength of the side channels as measured by entropy-based objectives, such as min-guess entropy. Our goal is to minimize the information leaks while guaranteeing a user-specified maximal acceptable performance overhead. We dub the decision version of this problem *Shannon mitigation*, and consider two variants, *deterministic* and *stochastic*. First, we show that the deterministic variant is NP-hard. However, we give a polynomial algorithm that finds an optimal solution from a restricted set. Second, for the stochastic variant, we develop an approach that uses optimization techniques specific to the entropy-based objective used. For instance, for min-guess entropy, we used mixed integer-linear programming. We apply the algorithm to a threat model where the attacker gets to make *functional observations*, that is, where she observes the running time of the program for the same secret value combined with different public input values. Existing mitigation approaches do not give confidentiality or performance guarantees for this threat model. We evaluate our tool Schmit on a number of micro-benchmarks and real-world applications with different entropy-based objectives. In contrast to the existing mitigation approaches, we show that in the functional-observation threat model, Schmit is scalable and able to maximize confidentiality under the performance overhead bound.

1 Introduction

Information leaks through timing side channels remain a challenging problem [13,16,24,29,35,37,47]. A program leaks secret information through timing side channels if an attacker can deduce secret values (or their properties) by observing response times. We consider the problem of mitigating timing side channels. Unlike elimination techniques [7,31,46] that aim to completely remove timing leaks without considering the performance penalty, the goal of mitigation techniques [10,26,48] is to weaken the leaks, while keeping the penalty low.

We define the *Shannon mitigation* problem that decides whether there is a mitigation policy to achieve a lower bound on a given security entropy-based

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measure while respecting an upper bound on the performance overhead. Consider an example where the program-under-analysis has a secret variable with seven possible values, and has three different timing behaviors, each forming a cluster of secret values. It takes 1 second if the secret value is 1, it takes 5 seconds if the secret is between 2 and 5, and it takes 10 seconds if the secret value is 6 or 7. The *entropy-based measure* quantifies the remaining uncertainty about the secret after timing observations. Min-guess entropy [11,25,41] for this program is 1, because if the observed execution time is 1, the attacker guesses the secret in one try. A *mitigation policy* involves merging some timing clusters by introducing delays. A good solution might be to introduce a 9 second delay if the secret is 1, which merges two timing clusters. But, this might be disallowed by the budget on the performance overhead. Therefore, another solution must be found, such as introducing a 4 seconds delay when the secret is one.

We develop two variants of the Shannon mitigation problem: *deterministic* and *stochastic*. The mitigation policy of the deterministic variant requires us to move all secret values associated to an observation to another observation, while the policy of the stochastic variant allows us to move only a portion of secret values in an observation to another one. We show that the deterministic variant of the Shannon mitigation problem is intractable and propose a dynamic programming algorithm to approximate the optimal solution for the problem by searching through a restricted set of solutions. We develop an algorithm that reduces the problem in the stochastic variant to a well-known optimization problem that depends on the entropy-based measure. For instance, with min-guess entropy, the optimization problem is mixed integer-linear programming.

We consider a threat model where an attacker knows the public inputs (known-message attacks [26]), and furthermore, where the public input changes much more often than the secret inputs (for instance, secrets such as bank account numbers do not change often). As a result, for each secret, the attacker observes a timing function of the public inputs. We call this model *functional observations* of timing side channels.

We develop our tool Schmit that has three components: side channel discovery [45], search for the mitigation policy, and the policy enforcement. The side channel discovery builds the functional observations [45] and measures the entropy of secret set after the observations. The mitigation policy component includes the implementation of the dynamic programming and optimization algorithms. The enforcement component is a monitoring system that uses the program internals and functional observations to enforce the policy at runtime. To summarize, we make the following contributions:

- We formalize the *Shannon mitigation* problem with two variants and show that the complexity of finding deterministic mitigation policy is NP-hard.
- We describe two algorithms for synthesizing the mitigation policy: one is based on dynamic programming for the deterministic variant, that is in polynomial time and results in an approximate solution, and the other one solves the stochastic variant of the problem with optimization techniques.

– We consider a threat model that results in functional observations. On a set of micro-benchmarks, we show that existing mitigation techniques are not secure and efficient for this threat model.
– We evaluate our approach on five real-world Java applications. We show that SCHMIT is scalable in synthesizing mitigation policy within a few seconds and significantly improves the security (entropy) of the applications.

```
Example(int high, int low) {
int t_high = high, t_low = low;
 while (t_high > 0) {
  if (t_high % 2 == 1) {
   while (t_low > 0) {
    if (t_low % 2 == 1) {
     res += compute(t_low,t_high);}
    t_low = t_low >> 1;}}
  t_high = t_high >> 1;}
 return res;}
```

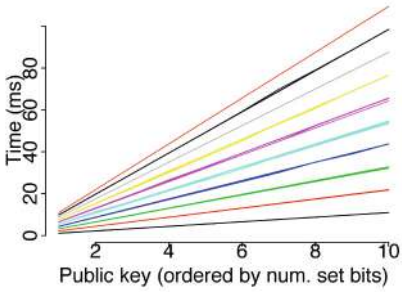


Fig. 1. (a) The example used in Sect. 2. (b) The timing functions for each secret value of the program.

2 Overview

First, we describe the threat model considered in this paper. Second, we describe our approach on a running example. Third, we compare the results of SCHMIT with the existing mitigation techniques [10,26,48] and show that SCHMIT achieves the highest entropy (i.e., best mitigation) for all three entropy objectives.

Threat Model. We assume that the attacker has access to the source code and the mitigation model, and she can sample the run-time of the application arbitrarily many times on her own machine. During an attack, she intends to guess a fixed secret of the target machine by observing the mitigated running time. Since we consider the attack models where the attacker knows the public inputs and the secret inputs are less volatile than public inputs, her observations are functional observations, where for each secret value, she learns a function from the public inputs to the running time.

Example 2.1. Consider the program shown in Fig. 1(a). It takes secret and public values as inputs. The running time depends on the number of set bits in both secret and public inputs. We assume that secret and public inputs can be between 1 and 1023. Figure 1(b) shows the running time of different secret values as timing functions, i.e., functions from the public inputs to the running time.

Side channel discovery. One can use existing tools to find the initial functional observations [44,45]. In Example 2.1, functional observations are $\mathcal{F} = \langle y, 2y, \ldots, 10y \rangle$ where y is a variable whose value is the number of set bits in the public input. The corresponding secret classes after this observation is $\mathcal{S}_{\mathcal{F}} = \langle 1_1, 1_2, 1_3, \ldots, 1_{10} \rangle$ where 1_n shows a set of secret values that have n set bits. The sizes of classes are $B = \{10, 45, 120, 210, 252, 210, 120, 45, 10, 1\}$. We use L_1-norm as metric to calculate the distance between the functional observations $\mathcal{F}$. This distance (penalty) matrix specifies extra performance overhead to move from one functional observation to another. With the assumption of uniform distributions over the secret input, Shannon entropy, guessing entropy, and the min-guessing entropy are 7.3, 90.1, and 1.0, respectively. These entropies are defined in Sect. 3 and measure the remaining entropy of the secret set after the observations. We aim to maximize the entropy measures, while keeping the performance overhead below a threshold, say 60% for this example.

Mitigation with Schmit. We use our tool SCHMIT to mitigate timing leaks of Example 2.1. The mitigation policy for the Shannon entropy objective is shown in Fig. 2(a). The policy results in two classes of observations. The policy requires to move functional observations $\langle y, 2y, \ldots, 5y \rangle$ to $\langle 6y \rangle$ and all other observations $\langle 7y, 8y, 9y \rangle$ to $\langle 10y \rangle$. To enforce this policy, we use a monitoring system at runtime. The monitoring system uses a decision tree model of the initial functional observations. The decision tree model characterizes each functional observation with associated program internals such as method calls or basic block invocations [43,44]. The decision tree model for the Example 2.1 is shown in Fig. 2(b). The monitoring system records program internals and matches it with the decision tree model to detect the current functional observation. Then, it adds delays, if necessary, to the execution time in order to enforce the mitigation policy. With this method, the mitigated functional observation is $\mathcal{G} = \langle 6y, 10y \rangle$ and the secret

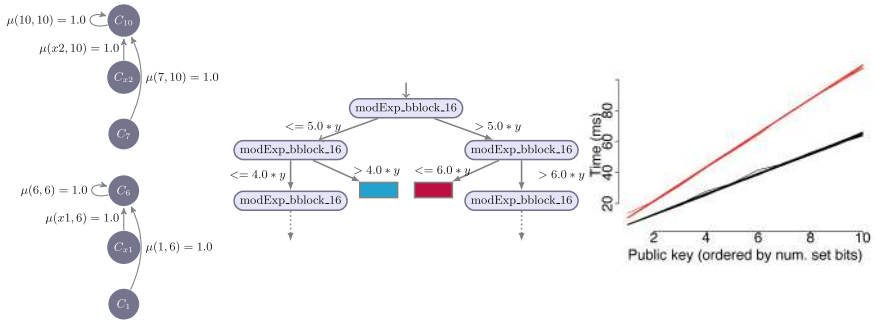


Fig. 2. (a) Mitigation policy calculation with deterministic algorithm (left). The observations $x1$ and $x2$ stands for all observations from $C_2 - C_5$ and from $C_8 - C_9$, resp.; (b) Leaned discriminant decision tree (center): it characterizes the functional clusters of Fig. 1(b) with internals of the program in Fig. 1(a); and (c) observations (right) after the mitigation by SCHMIT results in two classes of observations.

class is $\mathcal{S}_\mathcal{G} = \langle\{1_1, 1_2, 1_3, 1_4, 1_5, 1_6\}, \{1_7, 1_8, 1_9, 1_{10}\}\rangle$ as shown in Fig. 2 (c). The performance overhead of this mitigation is 43.1%. The Shannon, guessing, and min-guess entropies have improved to 9.7, 459.6, and 193.5, respectively.

Comparison with state of the art. We compare our mitigation results to black-box mitigation scheme [10] and bucketing [26]. *Black-box double scheme technique.* We use the double scheme technique [10] to mitigate the leaks of Example 2.1. This mitigation uses a prediction model to release events at scheduled times. Let us consider the prediction for releasing the event i at N-th epoch with $S(N, i) = \max(inp_i, S(N, i-1)) + p(N)$, where inp_i is the time arrival of the i-th request, $S(N, i-1)$ is the prediction for the request $i-1$, and $p(N) = 2^{N-1}$ models the basis for the prediction scheme at N-th epoch. We assume that the request are the same type and the sequence of public input requests for each secret are received in the beginning of epoch $N = 1$. Figure 3(a) shows the functional observations after applying the predictive mitigation. With this mitigation, the classes of observations are $\mathcal{S}_\mathcal{G} = \langle 1_1, \{1_2, 1_3\}, \{1_4, 1_5, 1_6, 1_7\}, \{1_8, 1_9, 1_{10}\}\rangle$. The number of classes of observations is reduced from 10 to 4. The performance overhead is 39.9%. The Shannon, guessing, and min-guess entropies have increased to 9.00, 321.5, and 5.5, respectively. *Bucketing.* We consider the mitigation approach with buckets [26]. For Example 2.1, if the attacker does not know the public input (unknown-message attacks [26]), the observations are $\{1.1, 2.1, 3.3, \cdots, 9.9, 10.9, \cdots, 109.5\}$ as shown in Fig. 3(b). We apply the bucketing algorithm in [26] for this observations, and it finds two buckets $\{37.5, 109.5\}$ shown with the red lines in Fig. 3(b). The bucketing mitigation requires to move the observations to the closet bucket. Without functional observations, there are 2 classes of observations. However, with functional observations, there are more than 2 observations. Figure 3(c) shows how the pattern of observations are leaking through functional side channels. There are 7 classes of observations: $\mathcal{S}_\mathcal{G} = \langle\{1_1, 1_2, 1_3\}, \{1_4\}, \{1_5\}, \{1_6\}, \{1_7\}, \{1_8\}, \{1_9\}, \{1_{10}\}\rangle$. The Shannon, guessing, and min-guess entropies are 7.63, 102.3, and 1.0, respectively.

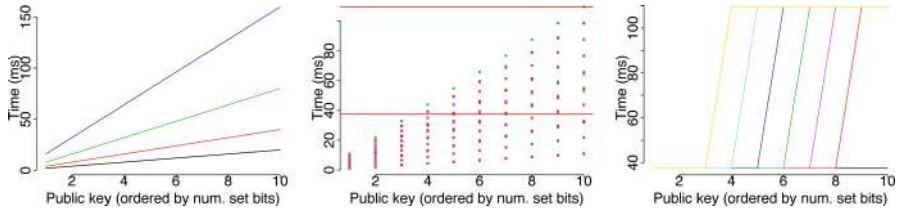


Fig. 3. (a) The execution time after mitigation using the double scheme technique [10]. There are four classes of functional observations after the mitigation. (b) Mitigation with bucketing [26]. All observations require to move to the closet red line. (c) Functional observations distinguish 7 classes of observations after mitigating with bucketing.

Overall, SCHMIT achieves the higher entropy measures for all three objectives under the performance overhead of 60%.

3 Preliminaries

For a finite set Q, we use $|Q|$ for its cardinality. A *discrete probability distribution*, or just distribution, over a set Q is a function $d : Q \to [0, 1]$ such that $\sum_{q \in Q} d(q) = 1$. Let $\mathcal{D}(Q)$ denote the set of all discrete distributions over Q. We say a distribution $d \in \mathcal{D}(Q)$ is a *point distribution* if $d(q)=1$ for a $q \in Q$. Similarly, a distribution $d \in \mathcal{D}(Q)$ is *uniform* if $d(q)=1/|Q|$ for all $q \in Q$.

Definition 1 (Timing Model). *The timing model of a program $\mathcal{P}$ is a tuple $[\![\mathcal{P}]\!] = (X, Y, \mathcal{S}, \delta)$ where $X = \{x_1, \ldots, x_n\}$ is the set of secret-input variables, $Y = \{y_1, \ldots, y_m\}$ is the set of public-input variables, $\mathcal{S} \subseteq \mathbb{R}^n$ is a finite set of secret-inputs, and $\delta : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}_{\geq 0}$ is the execution-time function of the program over the secret and public inputs.*

We assume that the adversary knows the program and wishes to learn the value of the secret input. To do so, for some fixed secret value $s \in \mathcal{S}$, the adversary can invoke the program to estimate (to an arbitrary precision) the execution time of the program. If the set of public inputs is empty, i.e. $m = 0$, the adversary can only make *scalar observations* of the execution time corresponding to a secret value. In the more general setting, however, the adversary can arrange his observations in a functional form by estimating an approximation of the *timing function* $\delta(s) : \mathbb{R}^m \to \mathbb{R}_{\geq 0}$ of the program.

A *functional observation* of the program $\mathcal{P}$ for a secret input $s \in \mathcal{S}$ is the function $\delta(s) : \mathbb{R}^m \to \mathbb{R}_{\geq 0}$ defined as $\mathbf{y} \in \mathbb{R}^m \mapsto \delta(s, \mathbf{y})$. Let $\mathcal{F} \subseteq [\mathbb{R}^m \to \mathbb{R}_{\geq 0}]$ be the finite set of all functional observations of the program $\mathcal{P}$. We define an order $\prec$ over the functional observations $\mathcal{F}$: for $f, g \in \mathcal{F}$ we say that $f \prec g$ if $f(y) \leq g(y)$ for all $y \in \mathbb{R}^m$.

The set $\mathcal{F}$ characterizes an equivalence relation $\equiv_{\mathcal{F}}$, namely secrets with equivalent functional observations, over the set $\mathcal{S}$, defined as following: $s \equiv_{\mathcal{F}} s'$ if there is an $f \in \mathcal{F}$ such that $\delta(s) = \delta(s') = f$. Let $\mathcal{S}_{\mathcal{F}} = \langle S_1, S_2, \ldots, S_k \rangle$ be the quotient space of $\mathcal{S}$ characterized by the observations $\mathcal{F} = \langle f_1, f_2, \ldots, f_k \rangle$. We write $\mathcal{S}_f$ for the secret set $S \in \mathcal{S}_{\mathcal{F}}$ corresponding to the observations $f \in \mathcal{F}$. Let $\mathcal{B} = \langle B_1, B_2, \ldots, B_k \rangle$ be the size of observational equivalence class in $\mathcal{S}_{\mathcal{F}}$, i.e. $B_i = |\mathcal{S}_{f_i}|$ for $f_i \in \mathcal{F}$ and let $B = |\mathcal{S}| = \sum_{i=1}^{k} B_i$.

Shannon entropy, guessing entropy, and min-guess entropy are three prevalent information metrics to quantify information leaks in programs. Köpf and Basin [25] characterize expressions for various information-theoretic measures on information leaks when there is a uniform distribution on $\mathcal{S}$ given below.

Proposition 1 (Köpf and Basin [25]). *Let $\mathcal{F} = \langle f_1, \ldots, f_k \rangle$ be a set of observations and let $\mathcal{S}$ be the set of secret values. Let $\mathcal{B} = \langle B_1, \ldots, B_k \rangle$ be the*

corresponding size of secret set in each class of observation and $B = \sum_{i=1}^{k} B_i$. *Assuming a uniform distribution on* $\mathcal{S}$, *entropies can be characterized as:*

1. **Shannon Entropy:** $\mathsf{SE}(\mathcal{S}|\mathcal{F}) \stackrel{\text{def}}{=} (\frac{1}{B}) \sum_{1 \leq i \leq k} B_i \log_2(B_i)$,
2. **Guessing Entropy:** $\mathsf{GE}(\mathcal{S}|\mathcal{F}) \stackrel{\text{def}}{=} (\frac{1}{2B}) \sum_{1 \leq i \leq k} B_i^2 + \frac{1}{2}$, *and*
3. **Min-Guess Entropy:** $\mathsf{mGE}(\mathcal{S}|\mathcal{F}) \stackrel{\text{def}}{=} \min_{1 \leq i \leq k} \{(B_i + 1)/2\}$.

4 Shannon Mitigation Problem

Our goal is to mitigate the information leakage due to the timing side channels by adding synthetic delays to the program. An aggressive, but commonly-used, mitigation strategy aims to eliminate the side channels by adding delays such that every secret value yields a common functional observation. However, this strategy may often be impractical as it may result in unacceptable performance degradations of the response time. Assuming a well-known penalty function associated with the performance degradation, we study the problem of maximizing entropy while respecting a bound on the performance degradation. We dub the decision version of this problem Shannon mitigation.

Adding synthetic delays to execution-time of the program, so as to mask the side-channel, can give rise to new functional observations that correspond to upper-envelopes of various combinations of original observations. Let $\mathcal{F} = \langle f_1, f_2, \ldots, f_k \rangle$ be the set of functional observations. For $I \subseteq 1, 2, \ldots, k$, let $f_I = \mathbf{y} \in \mathbb{R}^m \mapsto \sup_{i \in I} f_i(\mathbf{y})$ be the functional observation corresponding to upper-envelope of the functional observations in the set I. Let $\mathcal{G}(\mathcal{F}) = \{f_I : I \neq \emptyset \subseteq \{1, 2, \ldots, k\}\}$ be the set of all possible functional observations resulting from the upper-envelope calculations. To change the observation of a secret value with functional observation f_i to a new observation f_I (we assume that $i \in I$), we need to add delay function $f_I^i : \mathbf{y} \in \mathbb{R}^m \mapsto f_I(y) - f_i(y)$.

Mitigation Policies. Let $\mathcal{G} \subseteq \mathcal{G}(\mathcal{F})$ be a set of admissible post-mitigation observations. A *mitigation policy* is a function $\mu : \mathcal{F} \to \mathcal{D}(\mathcal{G})$ that for each secret $s \in \mathcal{S}_f$ suggests the probability distribution $\mu(f)$ over the functional observations. We say that a mitigation policy is *deterministic* if for all $f \in \mathcal{F}$ we have that $\mu(f)$ is a point distribution. Abusing notations, we represent a deterministic mitigation policy as a function $\mu : \mathcal{F} \to \mathcal{G}$. The semantics of a mitigation policy recommends to a program analyst a probability $\mu(f)(g)$ to elevate a secret input $s \in \mathcal{S}_f$ from the observational class f to the class $g \in \mathcal{G}$ by adding $\max\{0, g(p) - f(p)\}$ units delay to the corresponding execution-time $\delta(s, p)$ for all $p \in Y$. We assume that the mitigation policies respect the order, i.e. for every mitigation policy μ and for all $f \in \mathcal{F}$ and $g \in \mathcal{G}$, we have that $\mu(f)(g) > 0$ implies that $f \prec g$. Let $M_{(\mathcal{F} \to \mathcal{G})}$ be the set of mitigation policies from the set of observational clusters $\mathcal{F}$ into the clusters $\mathcal{G}$.

For the functional observations $\mathcal{F} = \langle f_1, \ldots, f_k \rangle$ and a mitigation policy $\mu \in M_{(\mathcal{F} \to \mathcal{G})}$, the resulting observation set $\mathcal{F}[\mu] \subseteq \mathcal{G}$ is defined as:

$$\mathcal{F}[\mu] = \{g \in \mathcal{G} \ : \ \text{there exists } f \in \mathcal{F} \text{ such that } \mu(f)(g) > 0\}.$$

Since the mitigation policy is stochastic, we use average sizes of resulting observations to represent fitness of a mitigation policy. For $\mathcal{F}[\mu] = \langle g_1, g_2, \ldots, g_\ell \rangle$, we define their expected class sizes $\mathcal{B}_\mu = \langle C_1, C_2, \ldots, C_\ell \rangle$ as $C_i = \sum_{j=1}^{i} \mu(f_j)(f_i) \cdot B_j$ (observe that $\sum_{i=1}^{\ell} C_i = B$). Assuming a uniform distribution on $\mathcal{S}$, various entropies for the expected class size after applying a policy $\mu \in M_{(\mathcal{F} \to \mathcal{G})}$ can be characterized by the following expressions:

1. **Shannon Entropy:** $\mathsf{SE}(\mathcal{S}|\mathcal{F}, \mu) \stackrel{\text{def}}{=} (\frac{1}{B}) \sum_{1 \le i \le \ell} C_i \log_2(C_i)$,
2. **Guessing Entropy:** $\mathsf{GE}(\mathcal{S}|\mathcal{F}, \mu) \stackrel{\text{def}}{=} (\frac{1}{2B}) \sum_{1 \le i \le \ell} C_i^2 + \frac{1}{2}$, and
3. **Min-Guess Entropy:** $\mathsf{mGE}(\mathcal{S}|\mathcal{F}, \mu) \stackrel{\text{def}}{=} \min_{1 \le i \le \ell} \{(C_i + 1)/2\}$.

We note that the above definitions do not represent the expected entropies, but rather entropies corresponding to the expected cluster sizes. However, the three quantities provide bounds on the expected entropies after applying μ. Since Shannon and Min-Guess entropies are concave functions, from Jensen's inequality, we get that $\mathsf{SE}(\mathcal{S}|\mathcal{F}, \mu)$ and $\mathsf{mGE}(\mathcal{S}|\mathcal{F}, \mu)$ are upper bounds on expected Shannon and Min-Guess entropies. Similarly, $\mathsf{GE}(\mathcal{S}|\mathcal{F}, \mu)$, being a convex function, give a lower bound on expected guessing entropy.

We are interested in maximizing the entropy while respecting constraints on the overall performance of the system. We formalize the notion of performance by introducing performance penalties: there is a function $\pi : \mathcal{F} \times \mathcal{G} \to \mathbb{R}_{\ge 0}$ such that elevating from the observation $f \in \mathcal{F}$ to the functional observation $g \in \mathcal{G}$ adds an extra $\pi(f, g)$ performance overheads to the program. The expected performance penalty associated with a policy μ, $\pi(\mu)$, is defined as the probabilistically weighted sum of the penalties, i.e. $\sum_{f \in \mathcal{F}, g \in \mathcal{G} : f \prec g} |\mathcal{S}_f| \cdot \mu(f)(g) \cdot \pi(f, g)$. Now, we introduce our key decision problem.

Definition 2 (Shannon Mitigation). *Given a set of functional observations $\mathcal{F} = \langle f_1, \ldots, f_k \rangle$, a set of admissible post-mitigation observations $\mathcal{G} \subseteq \mathcal{G}(\mathcal{F})$, set of secrets $\mathcal{S}$, a penalty function $\pi : \mathcal{F} \times \mathcal{G} \to \mathbb{R}_{\ge 0}$, a performance penalty upper bound $\Delta \in \mathbb{R}_{\ge 0}$, and an entropy lower-bound $E \in \mathbb{R}_{\ge 0}$, the Shannon mitigation problem $\textsc{Shan}_{\mathcal{E}}(\mathcal{F}, \mathcal{G}, \mathcal{S}, \pi, E, \Delta)$, for a given entropy measure $\mathcal{E} \in \{\mathsf{SE}, \mathsf{GE}, \mathsf{mGE}\}$, is to decide whether there exists a mitigation policy $\mu \in M_{(\mathcal{F} \to \mathcal{G})}$ such that $\mathcal{E}(\mathcal{S}|\mathcal{F}, \mu) \ge E$ and $\pi(\mu) \le \Delta$. We define the deterministic Shannon mitigation variant where the goal is to find a deterministic such policy.*

5 Algorithms for Shannon Mitigation Problem

5.1 Deterministic Shannon Mitigation

We first establish the intractability of the deterministic variant.

Theorem 1. *Deterministic Shannon mitigation problem is NP-complete.*

Proof. It is easy to see that the deterministic Shannon mitigation problem is in NP: one can guess a certificate as a deterministic mitigation policy $\mu \in M_{(\mathcal{F} \to \mathcal{G})}$

and can verify in polynomial time that it satisfies the entropy and overhead constraints. Next, we sketch the hardness proof for the min-guess entropy measure by providing a reduction from the *two-way partitioning* problem [28]. For the Shannon entropy and guess entropy measures, a reduction can be established from the Shannon capacity problem [18] and the Euclidean sum-of-squares clustering problem [8], respectively.

Given a set $A = \{a_1, a_2, \ldots, a_k\}$ of integer values, the two-way partitioning problem is to decide whether there is a partition $A_1 \uplus A_2 = A$ into two sets A_1 and A_2 with equal sums, i.e. $\sum_{a \in A_1} a = \sum_{a \in A_2} a$. W.l.o.g assume that $a_i \leq a_j$ for $i \leq j$. We reduce this problem to a deterministic Shannon mitigation problem $\textsc{Shan}_{\mathsf{mGE}}(\mathcal{F}_A, \mathcal{G}_A, \mathcal{S}_A, \pi_A, E_A, \Delta_A)$ with k clusters $\mathcal{F}_A = \mathcal{G}_A = \langle f_1, f_2, \ldots, f_k \rangle$ with the secret set $\mathcal{S}_A = \langle S_1, S_2, \ldots, S_k \rangle$ such that $|S_i| = a_i$. If $\sum_{1 \leq i \leq k} a_i$ is odd then the solution to the two-way partitioning instance is trivially `no`. Otherwise, let $E_A = (1/2) \sum_{1 \leq i \leq k} a_i$. Notice that any deterministic mitigation strategy that achieves min-guess entropy larger than or equal to E_A must have at most two clusters. On the other hand, the best min-guess entropy value can be achieved by having just a single cluster. To avoid this and force getting two clusters corresponding to the two partitions of a solution to the two-way partitions problem instance A, we introduce performance penalties such that merging more than $k-2$ clusters is disallowed by keeping performance penalty $\pi_A(f, g) = 1$ and performance overhead $\Delta_A = k - 2$. It is straightforward to verify that an instance of the resulting min-guess entropy problem has a `yes` answer if and only if the two-way partitioning instance does. □

Since the deterministic Shannon mitigation problem is intractable, we design an approximate solution for the problem. Note that the problem is hard even if we only use existing functional observations for mitigation, i.e., $\mathcal{G} = \mathcal{F}$. Therefore, we consider this case for the approximate solution. Furthermore, we assume the following *sequential dominance* restriction on a deterministic policy μ: for $f, g \in \mathcal{F}$ if $f \prec g$ then either $\mu(f) \prec g$ or $\mu(f) = \mu(g)$. In other words, for any given $f \prec g$, f can not be moved to a higher cluster than g without having g be moved to that cluster. For example, Fig. 4(a) shows Shannon mitigation problem with four functional observations and all possible mitigation policies (we represent $\mu(f_i)(f_j)$ with $\mu(i, j)$). Figure 4(b) satisfies the sequential dominance restriction, while Fig. 4(c) does not.

The search for the deterministic policies satisfying the sequential dominance restriction can be performed efficiently using dynamic programming by effective use of intermediate results' memorizations.

Algorithm (1) provides a pseudocode for the dynamic programming solution to find a deterministic mitigation policy satisfying the sequential dominance. The key idea is to start with considering policies that produce a single cluster for subclasses P_i of the problem with the observation from $\langle f_1, \ldots, f_i \rangle$, and then compute policies producing one additional cluster in each step by utilizing the previously computed sub-problems and keeping track of the performance penalties. The algorithm terminates as soon as the solution of the current step respects the performance bound. The complexity of the algorithm is $O(k^3)$.

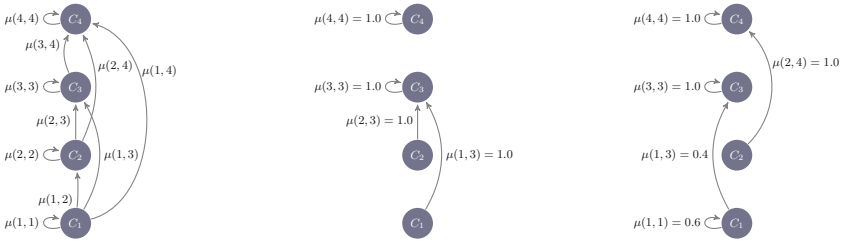


Fig. 4. (a). Example of Shannon mitigation problem with all possible mitigation policies for 4 classes of observations. (b,c) Two examples of the mitigation policies that results in 2 and 3 classes of observations.

5.2 Stochastic Shannon Mitigation Algorithm

Next, we solve the (stochastic) Shannon mitigation problem by posing it as an optimization problem. Consider the stochastic Shannon mitigation problem $\textsc{Shan}_{\mathcal{E}}$ $(\mathcal{F}, \mathcal{G} = \mathcal{F}, \mathcal{S}_{\mathcal{F}}, \pi, E, \Delta)$ with a stochastic policy $\mu : \mathcal{F} \to \mathcal{D}(\mathcal{G})$ and

Algorithm 1. Approximate Deterministic Shannon Mitigation

Input: The Shannon entropy problem $\textsc{Shan}_{MGE}(\mathcal{F}, \mathcal{G} = \mathcal{F}, \mathcal{S}_{\mathcal{F}}, \pi, E, \Delta)$
Output: The entropy table (T).

for $i = 1$ *to* k **do**
  $T(i,1) = \mathcal{E}(\bigcup_{j=1}^{i} S_j)$
  if $\sum_{1 \le j \le i} \pi(j,i)(B_j/B) \le \Delta$ **then** $\Pi(i,1) = \sum_{1 \le j \le i} \pi(j,i)(B_j/B)$
  else $\Pi(i,1) = \infty$
if $\Pi(k,1) < \infty$ **then return** T;
for $r = 2$ *to* k **do**
  for $i = 1$ *to* k **do**
    $\Omega(i,r) = \{j : 1 \le j < i \text{ and } \Pi(j, r-1) + \sum_{j < q \le i} \pi(q,i)(B_q/B) \le \Delta\}$
    if $\Omega \neq \emptyset$ **then** $T(i,r) = \max_{j \in \Omega(i,r)} \left(\min \left(T(j,r-1), \mathcal{E}(\bigcup_{q=j+1}^{i} S_q) \right) \right)$
    else $T(i,r) = -\infty$
    Let j be the index that maximizes $T(i,r)$
    if $\Omega \neq \emptyset$ **then** $\Pi(i,r) = \left(\Pi(j, r-1) + \sum_{j < q \le i} \pi(q,i)(B_q/B) \right)$
    else $\Pi(i,r) = \infty$
  if $\Pi(k,r) < \infty$ **then return** T;
return T;

$\mathcal{S}_{\mathcal{F}} = \langle S_1, S_2, \ldots, S_k \rangle$. The following program characterizes the optimization problem that solves the Shannon mitigation problem with stochastic policy.

Maximize $\mathcal{E}$, subject to:

1. $0 \leq \mu(f_i)(f_j) \leq 1$ for $1 \leq i \leq j \leq k$
2. $\sum_{i \leq j \leq k} \mu(f_i)(f_j) = 1$ for all $1 \leq i \leq k$.
3. $\sum_{i=1}^{k} \sum_{j=i}^{k} |S_i| \cdot \mu(f_i)(f_j) \cdot \pi(f_i, f_j) \leq \Delta$.
4. $C_j = \sum_{i=1}^{j} |S_i| \cdot \mu(f_i)(f_j)$ for $1 \leq j \leq k$.

Here, the objective function $\mathcal{E}$ is one of the following functions:

1. **Guessing Entropy** $\mathcal{E}_{GE} = \sum_{j=1}^{k} C_j^2$
2. **Min-Guess Entropy** $\mathcal{E}_{MGE} = \min_{1 \leq j \leq k} \{C_j \mid C_j > 0\}$
3. **Shannon Entropy** $\mathcal{E}_{SE} = \sum_{j=1}^{k} C_j \cdot \log_2(C_j)$

The linear constraints for the problem are defined as the following. The condition (1) and (2) express that μ provides a probability distributions, condition (3) provides restrictions regarding the performance constraint, and the condition (4) is the entropy specific constraint. The objective function of the optimization problem is defined based on the entropy criteria from $\mathcal{E}$. For the simplicity, we omit the constant terms from the objective function definitions. For the guessing entropy, the problem is an instance of linearly constrained quadratic optimization problem [33]. The problem with Shannon entropy is a non-linear optimization problem [12]. Finally, the optimization problem with min-guess entropy is an instance of mixed integer programming [32]. We evaluate the scalability of these solvers empirically in Sect. 6 and leave the exact complexity as an open problem. We show that the min-guess entropy objective function can be efficiently solved with the branch and bound algorithms [36]. Figure 4(b,c) show two instantiations of the mitigation policies that are possible for the stochastic mitigation.

6 Implementation Details

A. Environmental Setups. All timing measurements are conducted on an Intel NUC5i5RYH. We switch off JIT Compilation and run each experiment multiple times and use the mean running time. This helps to reduce the effects of environmental factors such as the Garbage Collections. All other analyses are conducted on an Intel i5-2.7 GHz machine.

B. Implementation of Side Channel Discovery. We use the technique presented in [45] for the side channel discovery. The technique applies the functional

data analysis [38] to create B-spline basis and fit functions to the vector of timing observations for each secret value. Then, the technique applies the functional data clustering [21] to obtain K classes of observations. We use the number of secret values in a cluster as the class size metric and the L_1 distance norm between the clusters as the penalty function.

C. Implementation of Mitigation Policy Algorithms. For the stochastic optimization, we encode the Shannon entropy and guessing entropy with linear constraints in Scipy [22]. Since the objective functions are non-linear (for the Shannon entropy) and quadratic (for the guessing entropy), Scipy uses sequential least square programming (SLSQP) [34] to maximize the objectives. For the stochastic optimization with the min-guess entropy, we encode the problem in Gurobi [19] as a mixed-integer programming (MIP) problem [32]. Gurobi solves the problem efficiently with branch-and-bound algorithms [1]. We use Java to implement the dynamic programming.

D. Implementation of Enforcement. The enforcement of mitigation policy is implemented in two steps. *First*, we use the initial timing functions and characterize them with program internal properties such as basic block calls. To do so, we use the decision tree learning approach presented in [45]. The decision tree model characterizes each functional observations with properties of program internals. *Second*, given the policy of mitigation, we enforce the mitigation policy with a monitoring system implemented on top of the Javassist [15] library. The monitoring system uses the decision tree model and matches the properties enabled during an execution with the tree model (detection of the current cluster). Then, it adds extra delays, based on the mitigation policy, to the current execution-time and enforces the mitigation policy. Note that the dynamic monitoring can result in a few micro-second delays. For the programs with timing differences in the order of micro-seconds, we transform source code using the decision tree model. The transformation requires manual efforts to modify and compile the new program. But, it adds negligible delays.

E. Micro-benchmark Results. Our goal is to compare different mitigation methods in terms of their security and performance. We examine the computation time of our tool SCHMIT in calculating the mitigation policies. See appendix for the relationships between performance bounds and entropy measures.

Applications: Mod_Exp applications [30] are instances of square-and-multiply modular exponentiation ($R = y^k \ mod \ n$) used for secret key operations in RSA [39]. Branch_and_Loop series consist of 6 applications where each application has conditions over secret values and runs a linear loop over the public values. The running time of the applications depend on the slope of the linear loops determined by the secret input.

Computation time comparisons: Fig. 5 shows the computation time for Branch_and _Loop applications (the applications are ordered in x-axis based on the discovered number of observational classes). For the min-guess entropy, we observe that both stochastic and dynamic programming approaches are efficient and fast as shown in Fig. 5(a). For the Shannon and guessing entropies,

Table 1. Micro-benchmark results. M_E and B_L stand for Mod_Exp and Branch_and_Loop applications. Legend: #**S**: no. of secret values, #**P**: no. of public values, Δ: Upper bound over performance penalty, ϵ: clustering parameter, #**K**: classes of observations before mitigation, #$\mathbf{K}_X$: classes of observations after mitigation with X technique, **mGE**: Min-guess entropy before mitigation, $\mathbf{mGE}_X$: Min-guess entropy after mitigation with X, $\mathbf{O}_X$: Performance overhead added after mitigation with X.

	Initial Characteristics						Double Scheme			Bucketing			Schmit (Determ.)			Schmit (Stoch.)		
App(s)	#S	#P	Δ	ϵ	#K	mGE	$\#K_{DS}$	mGE_{DS}	$O_{DS}(\%)$	$\#K_B$	mGE_B	$O_B(\%)$	K_D	$\#mGE_D$	$O_D(\%)$	$\#K_S$	mGE_S	$O_S(\%)$
M_E_1	32	32	0.5	1.0	1	16.5	1	16.5	0.0	1	16.5	0.0	1	16.5	0.0	1	16.5	0.0
M_E_2	64	64	0.5	1.0	2	16.5	1	32.5	5,221	1	32.5	27.6	1	32.5	21.4	1	32.5	21.4
M_E_3	128	128	0.5	2.0	2	32.5	1	64.5	5,407	1	64.5	33.9	1	64.5	22.7	1	64.5	22.7
M_E_4	256	256	0.5	2.0	4	10.5	1	128.5	6,679	1	128.5	30.7	1	128.5	28.3	1	128.5	28.3
M_E_5	512	512	0.5	5.0	23	1.0	1	256.5	7,294	2	128.5	50.0	1	256.5	31.0	1	253.0	30.3
M_E_6	1,024	1,024	0.5	8.0	40	1.0	1	512.5	7,822	20	1.0	34.5	2	27.5	46.7	5	85.5	50.0
B_L_1	25	50	0.5	10.0	4	3.0	3	3.0	73.0	3	3.0	17.5	2	5.5	26.1	2	6.5	34.9
B_L_2	50	50	0.5	10.0	8	3.0	4	3.0	61.3	5	3.0	21.9	2	10.5	45.3	2	13.0	45.3
B_L_3	100	50	0.5	20.0	16	3.0	4	8.0	42.4	8	3.0	33.4	2	20.5	48.3	2	21.5	50
B_L_4	200	50	0.5	20.0	32	3.0	6	3.0	36.9	16	3.0	28.7	2	48.0	48.7	2	50.5	49.7
B_L_5	400	50	0.5	20.0	64	3.0	8	3.0	35.4	32	3.0	27.2	3	65.5	32.0	2	100.5	50.0
B_L_6	800	50	0.5	20.0	125	3.0	12	8.0	37.8	29	3.0	52.5	3	133.0	34.6	2	200.5	49.6

the dynamic programming is scalable, while the stochastic mitigation is computationally expensive beyond 60 classes of observations as shown in Fig. 5(b,c).

Mitigation Algorithm Comparisons: Table 1 shows micro-benchmark results that compare the four mitigation algorithms with the two program series. Double scheme mitigation technique [10] does not provide guarantees on the performance overhead, and we can see that it is increased by more than 75 times for mod_exp_6. Double scheme method reduces the number of classes of observations. However, we observe that this mitigation has difficulty improving the min-guess entropy. Second, Bucketing algorithm [26] can guarantee the performance overhead, but it is not an effective method to improve the security of functional observations, see the examples mod_exp_6 and Branch_and_Loop_6. Third, in the algorithms, SCHMIT guarantees the performance to be below a certain bound, while it results in the highest entropy values. In most cases, the stochastic optimization technique achieves the highest min-entropy value. Here, we show the results with min-guess entropy measure. Also, we have strong evidences to show that SCHMIT achieves higher Shannon and guessing entropies. For example, in B_L_5, the initial Shannon entropy has improved from 2.72 to 6.62, 4.1, 7.56, and 7.28 for the double scheme, the bucketing, the stochastic, and the deterministic algorithms, respectively.

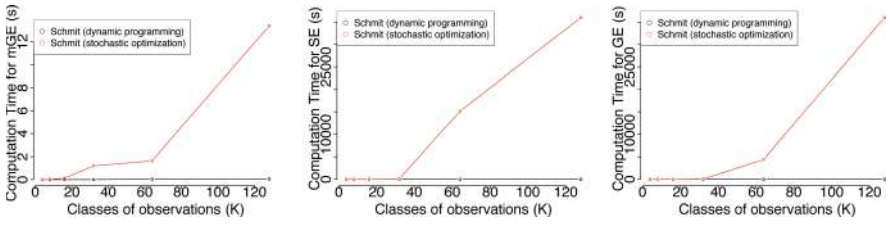


Fig. 5. Computation time for synthesizing mitigation policy over Branch_and_Loop applications. Computation time for min-guess entropy (a) takes only few seconds. Computation time for the Shannon entropy (b) and guessing entropy (c) are expensive using Stochastic optimization. We set time-out to be 10 hours.

7 Case Study

Research Question. Does SCHMIT scale well and improve the security of applications (entropy measures) within the given performance bounds?

Methodology. We use the deterministic and stochastic algorithms for mitigating the leaks. We show our results for the min-guess entropy, but other entropy measures can be applied as well. Since the task is to mitigate existing leakages, we assume that the secret and public inputs are given.

Objects of Study. We consider four real-world applications:

In the inset table, we show the basic characteristics of these benchmarks.

Application	Num methods	Num secret	Num public	ϵ	Initial clusters	Initial. Min-guess
GabFeed	573	1,105	65	6.50	34	1.0
Jetty	63	800	635	0.1	20	4.5
Java Verbal Expressions	61	2,000	10	0.02	9	50.5
Password Checker	6	20	2,620	0.05	6	1.0

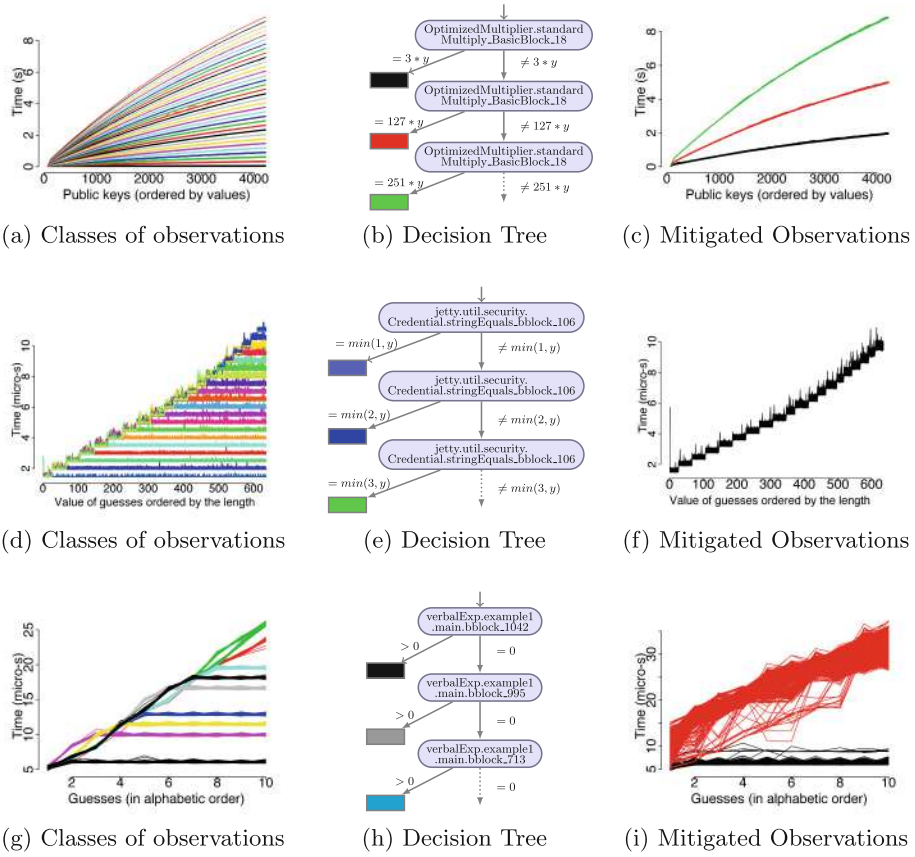
GabFeed is a chat server with 573 methods [4]. There is a side channel in the authentication part of the application where the application takes users' public keys and its own private key, and generating a common key [14]. The vulnerability leaks the number of set bits in the secret key. Initial functional observations are shown in Fig. 6a. There are 34 clusters and min-guess entropy is 1. We aim to maximize the min-guess entropy under the performance overhead of 50%.

Jetty. We mitigate the side channels in `util.security` package of Eclipse Jetty web server. The package has `Credential` class which had a timing side channel. This vulnerability was analyzed in [14] and fixed initially in [6]. Then, the developers noticed that the implementation in [6] can still leak information and fixed this issue with a new implementation in [5]. However, this new implementation is still leaking information [45]. We apply SCHMIT to mitigate this timing side channels. Initial functional observations is shown in Fig. 6d. There are 20 classes of observations and the initial min-guess entropy is 4.5. We aim to maximize the min-guess entropy under the performance overhead of 50%.

Java Verbal Expressions is a library with 61 methods that construct regular expressions [2]. There is a timing side channel in the library similar to password comparison vulnerability [3] if the library has secret inputs. In this case, starting from the initial character of a candidate expression, if the character matches with the regular expression, it slightly takes more time to respond the request than otherwise. This vulnerability can leak all the regular expressions. We consider regular expressions to have a maximum size of 9. There are 9 classes of observations and the initial min-guess entropy is 50.5. We aim to maximize the min-guess entropy under the performance overhead of 50%.

Password Checker. We consider the password matching example from loginBad program [9]. The password stored in the server is secret, and the user's guess is a public input. We consider 20 secret (lengths at most 6) and 2,620 public inputs. There are 6 different clusters, and the initial min-guess entropy is 1.

Findings for GabFeed. With the stochastic algorithm, SCHMIT calculates the mitigation policy that results in 4 clusters. This policy improves the min-guess entropy from 1 to 138.5 and adds an overhead of 42.8%. With deterministic algorithm, SCHMIT returns 3 clusters. The performance overhead is 49.7% and the min-guess entropy improves from 1 to 106. The user chooses the deterministic policy and enforces the mitigation. We apply CART decision tree learning and characterizes the classes of observations with GabFeed method calls as shown in



(a) Classes of observations (b) Decision Tree (c) Mitigated Observations

(d) Classes of observations (e) Decision Tree (f) Mitigated Observations

(g) Classes of observations (h) Decision Tree (i) Mitigated Observations

Fig. 6. Initial functional observations, decision tree, and the mitigated observations from left to right for Gabfeed, Jetty, and Verbal Expressions from top to bottom.

Fig. 6b. The monitoring system uses the decision tree model and automatically detects the current class of observation. Then, it adds extra delays based on the mitigation policy to enforce it. The results of the mitigation is shown in Fig. 6c. Answer for our research question. *Scalability*: It takes about 1 second to calculate the stochastic and the deterministic policies. *Security*: Stochastic and deterministic variants improve the min-guess entropy more than 100 times under the given performance overhead of 50%, respectively.

Findings for Jetty. The stochastic algorithm and the deterministic algorithm find the same policy that results in 1 cluster with 39.6% performance overhead. The min-guess entropy improves from 4.5 to 400.5. For the enforcement, SCHMIT first uses the initial clusterings and specifies their characteristics with program internals that result in the decision tree model shown in Fig. 6e. Since the response time is in the order of micro-seconds, we transform the source code using the decision tree model by adding extra counter variables. The results of

the mitigation is shown in Fig. 6f. *Scalability*: It takes less than 1 second to calculate the policies for both algorithms. *Security*: Stochastic and deterministic variants improve the min-guess entropy 89 times under the given performance overhead.

Findings for Java Verbal Expressions. For the stochastic algorithm, the policy results in 2 clusters, and the min-guess entropy has improved to 500.5. The performance overhead is 36%. For the dynamic programming, the policy results in 2 clusters. This adds 28% of performance overhead, while it improves the min-guess entropy from 50.5 to 450.5. The user chooses to use the deterministic policy for the mitigation. For the mitigation, we transform the source code using the decision tree model and add the extra delays based on the mitigation policy.

Findings for Password Matching. Both the deterministic and the stochastic algorithms result in finding a policy with 2 clusters where the min-guess entropy has improved from 1 to 5.5 with the performance overhead of 19.6%. For the mitigation, we transform the source code using the decision tree model and add extra delays based on the mitigation policy if necessary.

8 Related Work

Quantitative theory of information have been widely used to measure how much information is being leaked with side-channel observations [11,20,25,41]. Mitigation techniques increase the remaining entropy of secret sets leaked through the side channels, while considering the performance [10,23,26,40,48,49].

Köpf and Dürmuth [26] use a bucketing algorithm to partition programs' observations into intervals. With the unknown-message threat model, Köpf and Dürmuth [26] propose a dynamic programming algorithm to find the optimal number of possible observations under a performance penalty. The works [10,48] introduce different black-box schemes to mitigate leaks. In particular, Askarov et al. [10] show the quantizing time techniques, which permit events to release at scheduled constant slots, have the worst case leakage if the slot is not filled with events. Instead, they introduce the double scheme method that has a schedule of predictions like the quantizing approach, but if the event source fails to deliver events at the predicted time, the failure results in generating a new schedule in which the interval between predictions is doubled. We compare our mitigation technique with both algorithms throughout this paper.

Elimination of timing side channels is a common technique to guarantee the confidentiality of software [7,17,27,30,31,46]. The work [46] aims to eliminate side channels using static analysis enhanced with various techniques to keep the performance overheads low without guaranteeing the amounts of overhead. In contrast, we use dynamic analysis and allow a small amount of information to leak, but we guarantee an upper-bound on the performance overhead.

Machine learning techniques have been used for explaining timing differences between traces [42–44]. Tizpaz-Niari et al. [44] consider performance issues in softwares. They also cluster execution times of programs and then explain what

program properties distinguish the different functional clusters. We adopt their techniques for our security problem.

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Property Directed Self Composition

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Abstract. We address the problem of verifying *k-safety properties*: properties that refer to k interacting executions of a program. A prominent way to verify k-safety properties is by *self composition*. In this approach, the problem of checking k-safety over the original program is reduced to checking an "ordinary" safety property over a program that executes k copies of the original program in some order. The way in which the copies are composed determines how complicated it is to verify the composed program. We view this composition as provided by a *semantic self composition function* that maps each state of the composed program to the copies that make a move. Since the "quality" of a self composition function is measured by the ability to verify the safety of the composed program, we formulate the problem of inferring a self composition function together with the inductive invariant needed to verify safety of the composed program, where both are restricted to a given language. We develop a *property-directed* inference algorithm that, given a set of predicates, infers composition-invariant pairs expressed by Boolean combinations of the given predicates, or determines that no such pair exists. We implemented our algorithm and demonstrate that it is able to find self compositions that are beyond reach of existing tools.

1 Introduction

Many relational properties, such as noninterference [12], determinism [21], service level agreements [9], and more, can be reduced to the problem of k-safety. Namely, reasoning about k different traces of a program simultaneously. A common approach to verifying k-safety properties is by means of *self composition*, where the program is composed with k copies of itself [4,32]. A state of the composed program consists of the states of each copy, and a trace naturally corresponds to k traces of the original program. Therefore, k-safety properties of the original program become ordinary safety properties of the composition, hence reducing k-safety verification to ordinary safety. This enables reasoning about k-safety properties using any of the existing techniques for safety verification such as Hoare logic [20] or model checking [7].

While self composition is sound and complete for k-safety, its applicability is questionable for two main reasons: (i) considering several copies of the program greatly increases the state space; and (ii) the way in which the different copies are composed when reducing the problem to safety verification affects the complexity of the resulting self composed program, and as such affects the complexity of verifying it. Improving the applicability of self composition has been the topic of many

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works [2,14,18,26,30,33]. However, most efforts are focused on compositions that are pre-defined, or only depend on syntactic similarities.

In this paper, we take a different approach; we build upon the observation that by choosing the "right" composition, the verification can be greatly simplified by leveraging "simple" correlations between the executions. To that end, we propose an algorithm, called PDSC, for inferring a *property directed* self composition. Our approach uses a *dynamic* composition, where the composition of the different copies can change during verification, directed at simplifying the verification of the composed program.

Compositions considered in previous work differ in the order in which the copies of the program execute: either synchronously, asynchronously, or in some mix of the two [3,14,34]. To allow general compositions, we define a *composition function* that maps every state of the composed program to the set of copies that are scheduled in the next step. This determines the order of execution for the different copies, and thus induces the self composed program. Unlike most previous works where the composition is pre-defined based on syntactic rules only, our composition is *semantic* as it is defined over the state of the composed program.

To capture the difficulty of verifying the composed program, we consider verification by means of inferring an inductive invariant, parameterized by a language for expressing the inductive invariant. Intuitively, the more expressive the language needs to be, the more difficult the verification task is. We then define the problem of inferring a composition function *together* with an inductive invariant for verifying the safety of the composed program, where both are restricted to a given language. Note that for a fixed language $\mathcal{L}$, an inductive invariant may exist for some composition function but not for another[1]. Thus, the restriction to $\mathcal{L}$ defines a target for the inference algorithm, which is now directed at finding a composition that admits an inductive invariant in $\mathcal{L}$.

Example 1. To demonstrate our approach, consider the program in Fig. 1. The program inserts a new value into an array. We assume that the array A and its length len are "low"-security variables, while the inserted value h is "high"-security. The first loop finds the location in which h will be inserted. Note that the number of iterations depends on the value of h. Due to that, the second loop executes to ensure that the output i (which corresponds to the number of iterations) does not leak sensitive data. As an example, we emphasize that without the second loop, i could leak the location of h in A. To express the property that i does not leak sensitive data, we use the 2-safety property that in any two executions, if the inputs A and len are the same, so is the output i.

To verify the 2-safety property, consider two copies of the program. Let the language $\mathcal{L}$ for verifying the self composition be defined by the predicates depicted in Fig. 1. The most natural self composition to consider is a lock-step composition, where the copies execute synchronously. However, for such a composition the composed program may reach a state where, for example, $i_1 = i_2 + 1$. This occurs when the first copy exists the first loop, while the second copy is still executing it. Since the language cannot express this correlation between the two copies, no inductive invariant suffices to verify that $i_1 = i_2$ when the program terminates.

[1] See the extended version [29] for an example that requires a non-linear inductive invariant with a composition that is based on the control structure but has a linear invariant with another.

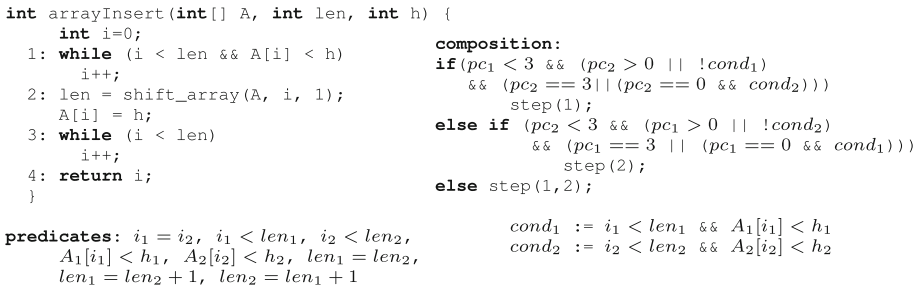

Fig. 1. Constant-time insert to an array.

In contrast, when verifying the 2-safety property, PDSC directs its search towards a composition function for which an inductive invariant in $\mathcal{L}$ does exist. As such, it infers the composition function depicted in Fig. 1, as well as an inductive invariant in $\mathcal{L}$. The invariant for this composition implies that $i_1 = i_2$ at every state.

As demonstrated by the example, PDSC focuses on logical languages based on predicate abstraction [17], where inductive invariants can be inferred by model checking. In order to infer a composition function that admits an inductive invariant in $\mathcal{L}$, PDSC starts from a default composition function, and modifies its definition based on the reasoning performed by the model checker during verification. As the composition function is part of the verified model (recall that it is defined over the program state), different compositions are part of the state space explored by the model checker. As a result, a key ingredient of PDSC is identifying "bad" compositions that prevent it from finding an inductive invariant in $\mathcal{L}$. It is important to note that a naive algorithm that tries all possible composition functions has a time complexity $O(2^{2^{|\mathcal{P}|}})$, where $\mathcal{P}$ is the set of predicates considered. However, integrating the search for a composition function into the model checking algorithm allows us to reduce the time complexity of the algorithm to $2^{O(|\mathcal{P}|)}$, where we show that the problem is in fact PSPACE-hard.[2]

We implemented PDSC using SEAHORN [19], Z3 [25] and SPACER [22] and evaluated it on examples that demonstrate the need for nontrivial semantic compositions. Our results clearly show that PDSC can solve complex examples by inferring the required composition, while other tools cannot verify these examples. We emphasize that for these particular examples, lock-step composition is not sufficient. We also evaluated PDSC on the examples from [26,30] that are proven with the trivial lock-step composition. On these examples, PDSC is comparable to state of the art tools.

Related Work. This paper addresses the problem of verifying k-safety properties (also called hyperproperties [8]) by means of self composition. Other approaches tackle the problem without self-composition, and often focus on more specific properties, most noticeably the 2-safety noninterference property (e.g. [1,33]). Below we focus on works that use self-composition.

[2] Proofs of the claims made in this paper can be found in the extended version [29].

Previous work such as [2–4,14,15,32] considered self composition (also called product programs) where the composition function is constant and set a-priori, using syntax-based hints. While useful in general, such self compositions may sometimes result in programs that are too complex to verify. This is in contrast to our approach, where the composition function is evolving during verification, and is adapted to the capabilities of the model checker.

The work most closely related to ours is [30] which introduces Cartesian Hoare Logic (CHL) for verification of k-safety properties, and designs a verification framework for this logic. This work is further improved in [26]. These works search for a proof in CHL, and in doing so, implicitly modify the composition. Our work infers the composition explicitly and can use off-the-shelf model checking tools. More importantly, when loops are involved both [30] and [26] use lock-step composition and align loops syntactically. Our algorithm, in contrast, does not rely on syntactic similarities, and can handle loops that cannot be aligned trivially.

There have been several results in the context of harnessing Constraint Horn Clauses (CHC) solvers for verification of relational properties [11,24]. Given several copies of a CHC system, a product CHC system that synchronizes the different copies is created by a syntactical analysis of the rules in the CHC system. These works restrict the synchronization points to CHC predicates (i.e., program locations), and consider only one synchronization (obtained via transformations of the system of CHCs). On the other hand, our algorithm iteratively searches for a good synchronization (composition), and considers synchronizations that depend on program state.

Equivalence Checking and Regression Verification. Equivalence checking is another closely related research field, where a composition of several programs is considered. As an example, equivalence checking is applied to verify the correctness of compiler optimizations [10,18,28,34]. In [28] the composition is determined by a brute-force search for possible synchronization points. While this brute-force search resembles our approach for finding the correct composition, it is not guided by the verification process. The works in [10,18] identify possible synchronization points syntactically, and try to match them during the construction of a simulation relation between programs.

Regression verification also requires the ability to show equivalence between different versions of a program [15,16,31]. The problem of synchronizing unbalanced loops appears in [31] in the form of unbalanced recursive function calls. To allow synchronization in such cases, the user can specify different unrolling parameters for the different copies. In contrast, our approach relies only on user supplied predicates that are needed to establish correctness, while synchronization is handled automatically.

2 Preliminaries

In this paper we reason about programs by means of the transition systems defining their semantics. A transition system is a tuple $T = (S, R, F)$, where S is a set of states, $R \subseteq S \times S$ is a transition relation that specifies the steps in an execution of the program, and $F \subseteq S$ is a set of *terminal states* $F \subseteq S$ such that every terminal state $s \in F$ has an outgoing transition to itself and no additional transitions (terminal states allow us to

reason about pre/post specifications of programs). An *execution* or *trace* $\pi = s_0, s_1, \ldots$ is a (finite or infinite) sequence of states such that for every $i \geq 0$, $(s_i, s_{i+1}) \in R$. The execution is *terminating* if there exists $0 \leq i \leq |\pi|$ such that $s_i \in F$. In this case, the suffix of the execution is of the form $s_i, s_i, \ldots$ and we say that π ends at s_i.

As usual, we represent transition systems using logical formulas over a set of variables, corresponding to the program variables. We denote the set of variables by $\mathcal{V}$. The set of terminal states is represented by a formula over $\mathcal{V}$ and the transition relation is represented by a formula over $\mathcal{V} \uplus \mathcal{V}'$, where $\mathcal{V}$ represents the pre-state of a transition and $\mathcal{V}' = \{v' \mid v \in \mathcal{V}\}$ represents its post-state. In the sequel, we use sets of states and their symbolic representation via formulas interchangeably.

Safety and Inductive Invariants. We consider safety properties defined via pre/post conditions.[3] A *safety property* is a pair $(pre, post)$ where $pre, post$ are formulas over $\mathcal{V}$, representing subsets of S, denoting the pre- and post-condition, respectively. T *satisfies* $(pre, post)$, denoted $T \models (pre, post)$, if every terminating execution π of T that starts in a state s_0 such that $s_0 \models pre$ ends in a state s such that $s \models post$. In other words, for every state s that is reachable in T from a state in *pre* we have that $s \models F \rightarrow post$.

A prominent way to verify safety properties is by finding an inductive invariant. An *inductive invariant* for a transition system T and a safety property $(pre, post)$ is a formula Inv such that(1) $pre \Rightarrow Inv$ (initiation), (2) $Inv \wedge R \Rightarrow Inv'$ (consecution), and (3) $Inv \Rightarrow (F \rightarrow post)$ (safety), where $\varphi \Rightarrow \psi$ denotes the validity of $\varphi \rightarrow \psi$, and φ' denotes $\varphi(\mathcal{V}')$, i.e., the formula obtained after substituting every $v \in \mathcal{V}$ by the corresponding $v' \in \mathcal{V}$. If there exists such an inductive invariant, then $T \models (pre, post)$.

k-safety. A *k-safety property* refers to k interacting executions of T. Similarly to an ordinary property, it is defined by $(pre, post)$, except that *pre* and *post* are defined over $\mathcal{V}^1 \uplus \ldots \uplus \mathcal{V}^k$ where $\mathcal{V}^i = \{v^i \mid v \in \mathcal{V}\}$ denotes the ith copy of the program variables. As such, *pre* and *post* represent sets of k-tuples of program states (*k-states* for short): for a k-tuple $(s_1, \ldots, s_k)$ of states and a formula φ over $\mathcal{V}^1 \uplus \ldots \uplus \mathcal{V}^k$, we say that $(s_1, \ldots, s_k) \models \varphi$ if φ is satisfied when for each i, the assignment of $\mathcal{V}^i$ is determined by s_i. We say that T *satisfies* $(pre, post)$, denoted $T \models^k (pre, post)$, if for every k terminating executions $\pi^1, \ldots, \pi^k$ of T that start in states $s_1, \ldots, s_k$, respectively, such that $(s_1, \ldots, s_k) \models pre$, it holds that they end in states $t_1, \ldots, t_k$, respectively, such that $(t_1, \ldots, t_k) \models post$.

For example, the *non interference* property may be specified by the following 2-safety property: $pre = \bigwedge_{v \in \mathrm{LowIn}} v^1 = v^2$, $post = \bigwedge_{v \in \mathrm{LowOut}} v^1 = v^2$ where LowIn and LowOut denote subsets of the program inputs, resp. outputs, that are considered "low security" and the rest are classified as "high security". This property asserts that every 2 terminating executions that start in states that agree on the "low security" inputs end in states that agree on the low security outputs, i.e., the outcome does not depend on any "high security" input and, hence, does not leak secure information.

Checking k-safety properties reduces to checking ordinary safety properties by creating a *self composed program* that consists of k copies of the transition system, each

[3] Our results can be extended to arbitrary safety (and k-safety) properties by introducing "observable" states to which the property may refer.

with its own copy of the variables, that run in parallel in some way. Thus, the self composed program is defined over variables $\mathcal{V}^{\|k} = \mathcal{V}^1 \uplus \ldots \uplus \mathcal{V}^k$, where $\mathcal{V}^i = \{v^i \mid v \in \mathcal{V}\}$ denotes the variables associated with the ith copy. For example, a common composition is a *lock-step* composition in which the copies execute simultaneously. The resulting composed transition system $T^{\|k} = (S^{\|k}, R^{\|k}, F^{\|k})$ is defined such that $S^{\|k} = S \times \ldots \times S$, $F^{\|k} = \bigwedge_{i=1}^{k} F(\mathcal{V}^i)$ and $R^{\|k} = \bigwedge_{i=1}^{k} R(\mathcal{V}^j, \mathcal{V}^{j\prime})$. Note that $R^{\|k}$ is defined over $\mathcal{V}^{\|k} \uplus \mathcal{V}^{\|k\prime}$ (as usual). Then, the k-safety property $(pre, post)$ is satisfied by T if and only if an ordinary safety property $(pre, post)$ is satisfied by $T^{\|k}$. More general notions of *self composition* are investigated in Sect. 3.

3 Inferring Self Compositions for Restricted Languages of Inductive Invariants

Any self-composition is sufficient for reducing k-safety to safety, e.g., lock-step, sequential, synchronous, asynchronous, etc. However, the choice of the self-composition used determines the difficulty of the resulting safety problem. Different self composed programs would require different inductive invariants, some of which cannot be expressed in a given logical language.

In this section, we formulate the problem of inferring a self composition function such that the obtained self composed program may be verified with a given language of inductive invariants. We are, therefore, interested in inferring both the self composition function and the inductive invariant for verifying the resulting self composed program. We start by formulating the kind of self compositions that we consider.

In the sequel, we fix a transition system $T = (S, R, F)$ with a set of variables $\mathcal{V}$.

3.1 Semantic Self Composition

Roughly speaking, a k self composition of T consists of k copies of T that execute together in some order, where steps may interleave or be performed simultaneously. The order is determined by a self composition function, which may also be viewed as a scheduler that is responsible for scheduling a subset of the copies in each step. We consider *semantic* compositions in which the order may depend on the *states* of the different copies, as well as the correlations between them (as opposed to *syntactic* compositions that only depend on the control locations of the copies, but may not depend on the values of other variables):

Definition 1 (Semantic Self Composition Function). *A* semantic k self composition function *(k-composition function for short) is a function $f : S^k \to \mathbb{P}(\{1..k\})$, mapping each k-state to a* nonempty *set of copies that are to participate in the next step of the self composed program*[4].

[4] We consider *memoryless* composition functions. Compositions that depend on the history of the (joint) execution are supported via ghost state added to the program to track the history.

We represent a k-composition function f by a set of logical conditions, with a condition C_M for every nonempty subset $M \subseteq \{1..k\}$ of the copies. For each such $M \subseteq \{1..k\}$, the condition C_M is defined over $\mathcal{V}^{\|k} = \mathcal{V}^1 \uplus \ldots \uplus \mathcal{V}^k$, and hence it represents a set of k-states, with the meaning that all the k-states that satisfy C_M are mapped to M by f:

$$f(s_1, \ldots, s_k) = M \text{ if and only if } (s_1, \ldots, s_k) \models C_M.$$

To ensure that the function is well defined, we require that $(\bigvee_M C_M) \equiv \mathit{true}$, which ensures that every k-state satisfies at least one of the conditions. We also require that for every $M_1 \neq M_2$, $C_{M_1} \wedge C_{M_2} \equiv \mathit{false}$, hence every k-state satisfies at most one condition. Together these requirements ensure that the conditions induce a partition of the set of all k-states. In the sequel, we identify a k-composition function f with its symbolic representation via conditions $\{C_M\}_M$ and use them interchangeably.

Definition 2 (Composed Program). *Given a k-composition function f, represented via conditions C_M for every nonempty set $M \subseteq \{1..k\}$, we define the k* self composition *of T to be the transition system $T^f = (S^{\|k}, R^f, F^{\|k})$ over variables $\mathcal{V}^{\|k} = \mathcal{V}^1 \uplus \ldots \uplus \mathcal{V}^k$ defined as follows: $F^{\|k} = \bigwedge_{i=1}^k F^i$, where $F^i = F(\mathcal{V}^i)$, and*

$$R^f = \bigvee_{\emptyset \neq M \subseteq \{1..k\}} (C_M \wedge \varphi_M) \quad \textit{where} \quad \varphi_M = \bigwedge_{j \in M} R(\mathcal{V}^j, \mathcal{V}^{j\prime}) \wedge \bigwedge_{j \notin M} \mathcal{V}^j = \mathcal{V}^{j\prime}$$

Thus, in T^f, the set of states consists of k-states ($S^{\|k} = S \times \ldots \times S$), the terminal states are k-states in which all the individual states are terminal, and the transition relation includes a transition from $(s_1, \ldots, s_k)$ to $(s'_1, \ldots, s'_k)$ if and only if $f(s_1, \ldots, s_k) = M$ and $(\forall i \in M.\ (s_i, s'_i) \in R) \wedge (\forall i \notin M.\ s_i = s'_i)$. That is, every transition of T^f corresponds to a simultaneous transition of a subset M of the k copies of T, where the subset is determined by the self composition function f. If $f(s_1, \ldots, s_k) = M$, then for every $i \in M$ we say that i is *scheduled* in $(s_1, \ldots, s_k)$.

Example 2. A k self composition that runs the k copies of T sequentially, one after the other, corresponds to a k-composition function f defined by $f(s_1, \ldots, s_k) = \{i\}$ where $i \in \{1..k\}$ is the minimal index of a non-terminal state in $\{s_1, \ldots, s_k\}$. If all states in $\{s_1, \ldots, s_k\}$ are terminal then $i = k$ (or any other index). This is encoded as follows: for every $1 \leq i < k$, $C_{\{i\}} = \neg F^i \wedge \bigwedge_{j<i} F^j$, $C_{\{k\}} = \bigwedge_{j<k} F^j$ and $C_M = \mathit{false}$ for every other $M \subseteq \{1..k\}$.

Example 3. The lock-step composition that runs the k copies of T synchronously corresponds to a k-self composition function f defined by $f(s_1, \ldots, s_k) = \{1, \ldots, k\}$, and encoded by $C_{\{1,\ldots,k\}} = \mathit{true}$ and $C_M = \mathit{false}$ for every other $M \subseteq \{1..k\}$.

In order to ensure soundness of a reduction of k-safety to safety via self composition, one has to require that the self composition function does not "starve" any copy of the transition system that is about to terminate if it continues to execute. We refer to this requirement as *fairness*.

Definition 3 (Fairness). *A k-self composition function f is* fair *if for every k terminating executions $\pi^1, \ldots, \pi^k$ of T there exists an execution $\pi^{\|}$ of T^f such that for every copy $i \in \{1..k\}$, the projection of $\pi^{\|}$ to i is π^i.*

Note that by the definition of the terminal states of T^f, $\pi^{\|}$ as above is guaranteed to be terminating. We say that the ith copy *terminates* in $\pi^{\|}$ if $\pi^{\|}$ contains a k-state $(s_1, \ldots, s_k)$ such that $s_i \in F$. Fairness may be enforced in a straightforward way by requiring that whenever $f(s_1, \ldots, s_k) = M$, the set M includes no index i for which $s_i \in F$, unless all have terminated. Since we assume that terminal states may only transition to themselves, a weaker requirement that suffices to ensure fairness is that M includes at least one index i for which $s_i \notin F$, unless there is no such index.

The following claim is now straightforward:

Lemma 1. *Let T be a transition system, $(pre, post)$ a k-safety property, and f a fair k-composition function for T and $(pre, post)$. Then*

$$T \models^k (pre, post) \text{ iff } \; T^f \models (pre, post).$$

Proof (sketch). Every terminating execution of T^f corresponds to k terminating executions of T. Fairness of f ensures that the converse also holds.

To demonstrate the necessity of the fairness requirement, consider a (non-fair) self composition function f that maps every state to $\{1\}$. Then, regardless of what the actual transition system T does, the resulting self composition T^f satisfies every pre-post specification vacuously, as it never reaches a terminal state.

Remark 1. While we require the conditions $\{C_M\}_M$ defining a self composition function f to induce a partition of $S^{\|k}$ in order to ensure that f is well defined as a (total) function, the requirement may be relaxed in two ways. First, we may allow C_{M_1} and C_{M_2} to overlap. This will add more transitions and may make the task of verifying the composed program more difficult, but it maintains the soundness of the reduction. Second, it suffices that the conditions cover the set of *reachable states* of the composed program rather than the entire state space. These relaxations do not damage soundness. Technically, this means that f represented by the conditions is a relation rather than a function. We still refer to it as a function and write $f(s_1, \ldots, s_k) = M$ to indicate that $(s_1, \ldots, s_k) \models C_M$, not excluding the possibility that $(s_1, \ldots, s_k) \models M'$ for $M' \neq M$ as well. We note that as long as the language used to describe compositions is closed under Boolean operations, we can always extract from the conditions $\{C_M\}_M$ a function f'. This is done as follows: First, to prevent the overlap between conditions, determine an arbitrary total order $<$ on the sets $M \subseteq \{1..k\}$ and set $C'_M := C_M \wedge \bigwedge_{N<M} \neg C_N$. Second, to ensure that the conditions cover the entire state space, set $C'_{\{1..k\}} := C'_{\{1..k\}} \vee \neg(\bigvee_M C_M)$. It is easy to verify that f' defined by $\{C'_M\}_M$ is a total self composition function and that if f is fair, then so is f'.

3.2 The Problem of Inferring Self Composition with Inductive Invariant

Lemma 1 states the soundness of the reduction of k-safety to ordinary safety. Together with the ability to verify safety by means of an inductive invariant, this leads to a verification procedure. However, while soundness of the reduction holds for *any* self composition, an inductive invariant in a given language may exist for the composed program

resulting from some compositions but not from others. We therefore consider the self composition function and the inductive invariant together, as a pair, leading to the following definition.

Definition 4. *Let T be a transition system and $(pre, post)$ a k safety property. For a formula Inv over $\mathcal{V}^{\|k}$ and a self composition function f represented by conditions $\{C_M\}_M$, we say that (f, Inv) is a* composition-invariant *pair for T and $(pre, post)$ if the following conditions hold:*

- $pre \implies Inv$ *(initiation of Inv),*
- *for every* $\emptyset \neq M \subseteq \{1..k\}$, $Inv \wedge C_M \wedge \varphi_M \implies Inv'$ *(consecution of Inv for* R^f*),*
- $Inv \implies \left((\bigwedge_{j=1}^{k} F^j) \rightarrow post\right)$ *(safety of Inv),*
- $Inv \implies \bigvee_M C_M$ *(f covers the reachable states),*
- *for every* $\emptyset \neq M \subseteq \{1..k\}$, $C_M \wedge (\bigvee_{j=1}^{k} \neg F^j) \implies \bigvee_{j \in M} \neg F^j$ *(f is fair).*

As commented in Remark 1, we relax the requirement that $(\bigvee_M C_M) \equiv true$ to $Inv \implies \bigvee_M C_M$, thus ensuring that the conditions cover all the reachable states. Since the reachable states of T^f are determined by $\{C_M\}_M$ (which define f), this reveals the interplay between the self composition function and the inductive invariant. Furthermore, we do not require that $C_{M_1} \wedge C_{M_2} \equiv false$ for $M_1 \neq M_2$, hence a k-state may satisfy multiple conditions. As explained earlier, these relaxations do not damage soundness. Furthermore, if we construct from f a self composition function f' as described in Remark 1, Inv would be an inductive invariant for $T^{f'}$ as well.

Lemma 2. *If there exists a composition-invariant pair (f, Inv) for T and $(pre, post)$, then $T \models^k (pre, post)$.*

If we do not restrict the language in which f and Inv are specified, then the converse also holds. However, in the sequel we are interested in the ability to verify k-safety with a given language, e.g., one for which the conditions of Definition 4 belong to a decidable fragment of logic and hence can be discharged automatically.

Definition 5 (Inference in $\mathcal{L}$). *Let $\mathcal{L}$ be a logical language. The problem of inferring a composition-invariant pair in $\mathcal{L}$ is defined as follows. The input is a transition system T and a k-safety property $(pre, post)$. The output is a composition-invariant pair (f, Inv) for T and $(pre, post)$ (as defined in Definition 4), where $Inv \in \mathcal{L}$ and f is represented by conditions $\{C_M\}_M$ such that $C_M \in \mathcal{L}$ for every $\emptyset \neq M \subseteq \{1..k\}$. If no such pair exists, the output is "no solution".*

When no solution exists, it does not necessarily mean that $T \not\models^k (pre, post)$. Instead, it may be that the language $\mathcal{L}$ is simply not expressive enough. Unfortunately, for expressive languages (e.g., quantified formulas or even quantifier free linear integer arithmetic), the problem of inferring an inductive invariant alone is already undecidable, making the problem of inferring a composition-invariant pair undecidable as well:

Lemma 3. *Let $\mathcal{L}$ be closed under Boolean operations and under substitution of a variable with a value, and include equalities of the form $v = a$, where v is a variable and a is a value (of the same sort). If the problem of inferring an inductive invariant in $\mathcal{L}$ is undecidable, then so is the problem of inferring a composition-invariant pair in $\mathcal{L}$.*

For example, linear integer arithmetic satisfies the conditions of the lemma. This motivates us to restrict the languages of inductive invariants. Specifically, we consider languages defined by a finite set of predicates. We consider *relational* predicates, defined over $\mathcal{V}^{\|k} = \mathcal{V}^1 \uplus \ldots \uplus \mathcal{V}^k$. For a finite set of predicates $\mathcal{P}$, we define $\mathcal{L}_\mathcal{P}$ to be the set of all formulas obtained by Boolean combinations of the predicates in $\mathcal{P}$.

Definition 6 (Inference using predicate abstraction). *The problem of inferring a predicate-based composition-invariant pair is defined as follows. The input is a transition system T, a k-safety property $(pre, post)$, and a finite set of predicates $\mathcal{P}$. The output is the solution to the problem of inferring a composition-invariant pair for T and $(pre, post)$ in $\mathcal{L}_\mathcal{P}$.*

Remark 2. It is possible to decouple the language used for expressing the self composition function from the language used to express the inductive invariant. Clearly, different sets of predicates (and hence languages) can be assigned to the self composition function and to the inductive invariant. However, since inductiveness is defined with respect to the transitions of the composed system, which are in turn defined by the self composition function, if the language defining f is not included in the language defining Inv, the conditions C_M themselves would be over-approximated when checking the requirements of Definition 4 and therefore would incur a precision loss. For this reason, we use the same language for both.

Since the problem of invariant inference in $\mathcal{L}_\mathcal{P}$ is PSPACE-hard [23], a reduction from the problem of inferring inductive invariants to the problem of inferring composition-invariant pairs (similar to the one used in the proof of Lemma 3) shows that composition-invariant inference in $\mathcal{L}_\mathcal{P}$ is also PSPACE-hard:

Theorem 1. *Inferring a predicate-based composition-invariant pair is PSPACE-hard.*

4 Algorithm for Inferring Composition-Invariant Pairs

In this section, we present Property Directed Self-Composition, PDSC for short—our algorithm for tackling the composition-invariant inference problem for languages of predicates (Definition 6). Namely, given a transition system T, a k-safety property $(pre, post)$ and a finite set of predicates $\mathcal{P}$, we address the problem of finding a pair (f, Inv), where f is a self composition function and Inv is an inductive invariant for the composed transition system T^f obtained from f, and both of them are in $\mathcal{L}_\mathcal{P}$, i.e., defined by Boolean combinations of the predicates in $\mathcal{P}$.

We rely on the property that a transition system (in our case T^f) has an inductive invariant in $\mathcal{L}_\mathcal{P}$ if and only if its abstraction obtained using $\mathcal{P}$ is safe. This is because, the set of reachable abstract states is the strongest set expressible in $\mathcal{L}_\mathcal{P}$ that satisfies initiation and consecution. Given T^f, this allows us to use predicate abstraction to either obtain an inductive invariant in $\mathcal{L}_\mathcal{P}$ for T^f (if the abstraction of T^f is safe) or determine that no such inductive invariant exists (if an abstract counterexample trace is obtained). The latter indicates that a different self composition function needs to be considered. A naive realization of this idea gives rise to an iterative algorithm that starts from an

$f \leftarrow$ lockstep , $E \leftarrow \emptyset$, *Unreach* $\leftarrow$ *false*
while *(true)* **do**
  $(res, Inv, cex) \leftarrow$ `Abs_Reach`$(\mathcal{P}, T^f, pre, post, Unreach)$
  if $res =$ *safe* **then return** $(f, Inv(\mathcal{P}))$
  $(\hat{s}, M) \leftarrow$ `Last_Step`(cex)
  $E \leftarrow E \cup \{(\hat{s}, M)\}$
  while *(*`All_Excluded_Or_Starving`$(\hat{s}, E)$*)* **do**
    Unreach $\leftarrow$ *Unreach* $\vee \hat{s}$
    if *Unreach* $\wedge \varphi_{pre}(\mathcal{B}) \not\equiv$ *false* **then return** "no solution in $\mathcal{L}_{\mathcal{P}}$"
    $cex \leftarrow$ `Remove_Last_Step`(cex)
    $(\hat{s}, M) \leftarrow$ `Last_Step`(cex)
    $E \leftarrow E \cup \{(\hat{s}, M)\}$
  $f \leftarrow$ `Modify_SC`$(f, \hat{s}, E)$

Algorithm 1. PDSC: Property-Directed Self-Composition.

arbitrary initial composition function and in each iteration computes a new composition function. At the worst case such an algorithm enumerates all self composition functions defined in $\mathcal{L}_{\mathcal{P}}$, i.e., has time complexity $O(2^{2^{|\mathcal{P}|}})$. Importantly, we observe that, when no inductive invariant exists for some composition function, we can use the abstract counterexample trace returned in this case to (i) generalize and eliminate multiple composition functions, and (ii) identify that some abstract states must be unreachable if there is to be a composition-invariant pair, i.e., we "block" states in the spirit of *property directed reachability* [5,13]. This leads to the algorithm depicted in Algorithm 1 whose worst case time complexity is $2^{O(|\mathcal{P}|)}$. Next, we explain the algorithm in detail.

Finding an Inductive Invariant for a Given Composition Function Using Predicate Abstraction. We use predicate abstraction [17,27] to check if a given candidate composition function has a corresponding inductive invariant. This is done as follows. The abstraction of T^f using $\mathcal{P}$, denoted $A_{\mathcal{P}}(T^f)$, is a transition system $(\hat{S}, \hat{R})$ defined over variables $\mathcal{B}$, where $\mathcal{B} = \{b_p \mid p \in \mathcal{P}\}$ (we omit the terminal states). $\hat{S} = \{0,1\}^{\mathcal{B}}$, i.e., each abstract state corresponds to a valuation of the Boolean variables representing $\mathcal{P}$. An abstract state $\hat{s} \in \hat{S}$ represents the following set of states of T^f:

$$\gamma(\hat{s}) = \{s^{\|} \in S^{\|k} \mid \forall p \in \mathcal{P}.\ s^{\|} \models p \Leftrightarrow \hat{s}(b_p) = 1\}$$

We extend γ to sets of states and to formulas representing sets of states in the usual way. The abstract transition relation is defined as usual:

$$\hat{R} = \{(\hat{s}_1, \hat{s}_2) \mid \exists {s^{\|}}_1 \in \gamma(\hat{s}_1)\ \exists {s^{\|}}_2 \in \gamma(\hat{s}_2).\ ({s^{\|}}_1, {s^{\|}}_2) \in R^f\}$$

Note that the set of abstract states in $A_{\mathcal{P}}(T^f)$ does *not* depend on f.

Notation. We sometimes refer to an abstract state $\hat{s} \in \hat{S}$ as the formula $\bigwedge_{\hat{s}(b_p)=1} b_p \wedge \bigwedge_{\hat{s}(b_p)=0} \neg b_p$. For a formula $\psi \in \mathcal{L}_{\mathcal{P}}$, we denote by $\psi(\mathcal{B})$ the result of substituting each $p \in \mathcal{P}$ in ψ by the corresponding Boolean variable b_p. For the opposite direction, given

a formula ψ over $\mathcal{B}$, we denote by $\psi(\mathcal{P})$ the formula in $\mathcal{L}_\mathcal{P}$ resulting from substituting each $b_p \in \mathcal{B}$ in ψ by p. Therefore, $\psi(\mathcal{P})$ is a symbolic representation of $\gamma(\psi)$.

Every set defined by a formula $\psi \in \mathcal{L}_\mathcal{P}$ is precisely represented by $\psi(\mathcal{B})$ in the sense that $\gamma(\psi(\mathcal{B}))$ is equal to the set of states defined by ψ, i.e., $\psi(\mathcal{B})$ is a precise abstraction of ψ. For simplicity, we assume that the termination conditions as well as the pre/post specification can be expressed precisely using the abstraction, in the following sense:

Definition 7. *$\mathcal{P}$ is* adequate *for T and $(pre, post)$ if there exist $\varphi_{pre}, \varphi_{post}, \varphi_{F^i} \in \mathcal{L}_\mathcal{P}$ such that $\varphi_{pre} \equiv pre$, $\varphi_{post} \equiv post$ and $\varphi_{F^i} \equiv F^i$ (for every copy $i \in \{1..k\}$).*

The following lemma provides the foundation for our algorithm:

Lemma 4. *Let T be a transition system, $(pre, post)$ a k safety property, and $\mathcal{P}$ a finite set of predicates adequate for T and $(pre, post)$. For a self composition function f defined via conditions $\{C_M\}_M$ in $\mathcal{L}_\mathcal{P}$, there exists an inductive invariant Inv in $\mathcal{L}_\mathcal{P}$ such that (f, Inv) is a composition-invariant pair for T and $(pre, post)$ if and only if the following three conditions hold:*

S1 *All reachable states of $A_\mathcal{P}(T^f)$ from $\varphi_{pre}(\mathcal{B})$ satisfy $(\bigwedge_{i=1}^{k} \varphi_{F^i}(\mathcal{B})) \rightarrow \varphi_{post}(\mathcal{B})$,*
S2 *All reachable states of $A_\mathcal{P}(T^f)$ from $\varphi_{pre}(\mathcal{B})$ satisfy $\bigvee_M C_M(\mathcal{B})$, and*
S3 *For every $\emptyset \neq M \subseteq \{1..k\}$, $C_M(\mathcal{B}) \wedge (\bigvee_{j=1}^{k} \neg\varphi_{F^j}(\mathcal{B})) \implies \bigvee_{j \in M} \neg\varphi_{F^j}(\mathcal{B})$.*

Furthermore, if the conditions hold, then the symbolic representation of the set of abstract states of $A_\mathcal{P}(T^f)$ reachable from $\varphi_{pre}(\mathcal{B})$ is a formula Inv over $\mathcal{B}$ such that $(f, Inv(\mathcal{P}))$ is a composition-invariant pair for T and $(pre, post)$.

Algorithm 1 starts from the lock-step self composition function (Line 1), which is fair[5], and constructs the next candidate f such that condition **S3** in Lemma 4 always holds (see discussion of `Modify_SC`). Thus, condition **S3** need not be checked explicitly.

Algorithm 1 checks whether conditions **S1** and **S2** hold for a given candidate composition function f by calling `Abs_Reach` (Line.3) – both checks are performed via a (non-)reachability check in $A_\mathcal{P}(T^f)$, checking whether a state violating $(\bigwedge_{i=1}^{k} \varphi_{F^i}(\mathcal{B})) \rightarrow \varphi_{post}(\mathcal{B})$ or $\bigvee_M C_M(\mathcal{B})$ is reachable from $\varphi_{pre}(\mathcal{B})$. Algorithm 1 maintains the abstract states that are not in $\bigvee_M C_M(\mathcal{B})$ by the formula *Unreach* defined over $\mathcal{B}$, which is initialized to *false* (as the lock-step composition function is defined for every state) and is updated in each iteration of Algorithm 1 to include the abstract states violating $\bigvee_M C_M(\mathcal{B})$. If no abstract state violating **S1** or **S2** is reachable, i.e., the conditions hold, then `Abs_Reach` returns the (potentially overapproximated) set of reachable abstract states, represented by a formula Inv over $\mathcal{B}$. In this case, by Lemma 4, $(f, Inv(\mathcal{P}))$ is a composition-invariant pair (line 4). Otherwise, an abstract counterexample trace is obtained. (We can of course apply bounded model checking to check if the counterexample is real; we omit this check as our focus is on the case where the system is safe.)

Remark 3. In practice, we do not construct $A_\mathcal{P}(T^f)$ explicitly. Instead, we use the *implicit predicate abstraction* approach [6].

[5] Any fair self composition can be chosen as the initial one; we chose lock-step since it is a good starting point in many applications.

Eliminating Self Composition Candidates Based on Abstract Counterexamples. An abstract counterexample to conditions **S1** or **S2** indicates that the candidate composition function f has no corresponding Inv. Violation of **S1** can only be resolved by changing f such that the abstract trace is no longer feasible. Violation of **S2** may, in principle, also be resolved by extending the definition of f such that it is defined for all the abstract states in the counterexample trace.

However, to prevent the need to explore both options, our algorithm maintains the following invariant for every candidate self composition function f that it constructs:

Claim. Every abstract state that is *not* in $\bigvee_M C_M(\mathcal{B})$ is not reachable w.r.t. the abstract composed program of *any* composition function that is part of a composition-invariant pair for T and $(pre, post)$.

This property clearly holds for the lock-step composition function, which the algorithm starts with, since for this composition, $\bigvee_M C_M(\mathcal{B}) \equiv true$. As we explain in Corollary 2, it continues to hold throughout the algorithm.

As a result of this property, whenever a candidate composition function f does not satisfy condition **S1** or **S2**, it is never the case that $\bigvee_M C_M(\mathcal{B})$ needs to be extended to allow the abstract states in cex to be reachable. Instead, the abstract counterexample obtained in violation of the conditions needs to be eliminated by modifying f.

Let $cex = \hat{s}_1, \ldots, \hat{s}_{m+1}$ be an abstract counterexample of $A_{\mathcal{P}}(T^f)$ such that $\hat{s}_1 \models \varphi_{pre}(\mathcal{B})$ and $\hat{s}_{m+1} \models (\bigwedge_{i=1}^{k} \varphi_{F^i}(\mathcal{B})) \wedge \neg\varphi_{post}(\mathcal{B})$ (violating **S1**) or $\hat{s}_{m+1} \models Unreach$ (violating **S2**). Any self composition f' that agrees with f on the states in $\gamma(\hat{s}_i)$ for every $\hat{s}_i$ that appears in cex has the same transitions in R^f and, hence, the same transitions in $\hat{R}$. It, therefore, exhibits the same abstract counterexample in $A_{\mathcal{P}}(T^{f'})$. Hence, it violates **S1** or **S2** and is not part of any composition-invariant pair.

Notation. Recall that f is defined via conditions $C_M \in \mathcal{L}_{\mathcal{P}}$. This ensures that for every abstract state $\hat{s}$, f is defined in the same way for all the states in $\gamma(\hat{s})$. We denote the value of f on the states in $\gamma(\hat{s})$ by $f(\hat{s})$ (in particular, $f(\hat{s})$ may be undefined). We get that $f(\hat{s}) = M$ if and only if $\hat{s} \models C_M(\mathcal{B})$.

Using this notation, to eliminate the abstract counterexample cex, one needs to eliminate at least one of the transitions in cex by changing the definition of $f(\hat{s}_i)$ for *some* $1 \leq i \leq m$. For a new candidate function f' this may be encoded by the disjunctive constraint $\bigvee_{i=1}^{m} f'(\hat{s}_i) \neq f(\hat{s}_i)$. However, we observe that a stronger requirement may be derived from cex based on the following lemma:

Lemma 5. *Let f be a self composition function and $cex = \hat{s}_1, \ldots, \hat{s}_{m+1}$ a counterexample trace in $A_{\mathcal{P}}(T^f)$ such that $\hat{s}_1 \models \varphi_{pre}(\mathcal{B})$ but $\hat{s}_{m+1} \models (\bigwedge_{i=1}^{k} \varphi_{F^i}(\mathcal{B})) \wedge \neg\varphi_{post}(\mathcal{B})$ or $\hat{s}_{m+1} \models Unreach$. Then for any self composition function f' such that $f'(\hat{s}_m) = f(\hat{s}_m)$, if $\hat{s}_m$ is reachable in $A_{\mathcal{P}}(T^{f'})$ from $\varphi_{pre}(\mathcal{B})$, then a counterexample trace to* **S1** *or* **S2** *exists.*

Corollary 1. *If there exists a composition-invariant pair (f', Inv'), then there is also one where $f'(\hat{s}_m) \neq f(\hat{s}_m)$.*

Therefore, we require that in the next self composition candidates the abstract state $\hat{s}_m$ must not be mapped to its current value in f, i.e., $f'(\hat{s}_m) \neq M$, where $f(\hat{s}_m) = M$[6].

Algorithm 1 accumulates these constraints in the set E (Line 6). Formally, the constraint $(\hat{s}, M) \in E$ asserts that C'_M must imply $\neg(\bigwedge_{\hat{s}(b_p)=1} p \wedge \bigwedge_{\hat{s}(b_p)=0} \neg p)$, and hence $f'(\hat{s}) \neq M$.

Identifying Abstract States that Must Be Unreachable. A new candidate self composition is constructed such that it satisfies all the constraints in E (thus ensuring that no abstract counterexample will re-appear). In the construction, we make sure to satisfy **S3** (fairness). Therefore, for every abstract state $\hat{s}$, we choose a value $f'(\hat{s})$ that satisfies the constraints in E and is *non-starving*: a value M is starving for $\hat{s}$ if $\hat{s} \models \bigvee_{j=1}^{k} \neg\varphi_{F^j}(\mathcal{B})$ but $\hat{s} \not\models \bigvee_{j \in M} \neg\varphi_{F^j}(\mathcal{B})$, i.e., some of the copies have not terminated in $\hat{s}$ but none of the non-terminating copies is scheduled. (Due to adequacy, a value M is starving for $\hat{s}$ if and only if it is starving for every $s^{\|} \in \gamma(\hat{s})$.)

If for some abstract state $\hat{s}$, all the non-starving values have already been excluded (i.e., $(\hat{s}, M) \in E$ for every non-starving M), we conclude that there is *no* f' such that $\hat{s}$ is reachable in $A_{\mathcal{P}}(T^{f'})$ and f' is part of a composition-invariant pair:

Lemma 6. *Let $\hat{s} \in \hat{S}$ be an abstract state such that for every $\emptyset \neq M \subseteq \{1..k\}$ either M is starving for $\hat{s}$ or $(\hat{s}, M) \in E$. Then, for every f' that satisfies* **S3***, if $A_{\mathcal{P}}(T^{f'})$ satisfies* **S1** *and* **S2***, then $\hat{s}$ is unreachable in $A_{\mathcal{P}}(T^{f'})$.*

Corollary 2. *If there exists a composition-invariant pair (f', Inv'), then $\hat{s}$ is unreachable in $A_{\mathcal{P}}(T^{f'})$.*

This is because no matter how the self composition function f' would be defined, $\hat{s}$ is guaranteed to have an outgoing abstract counterexample trace in $A_{\mathcal{P}}(T^{f'})$.

We, therefore, turn $f'(\hat{s})$ to be undefined. As a result, condition **S2** of Algorithm 4 requires that $\hat{s}$ will be unreachable in $A_{\mathcal{P}}(T^{f'})$. In Algorithm 1, this is enforced by adding $\hat{s}$ to *Unreach* (Line 8).

Every abstract state $\hat{s}$ that is added to *Unreach* is a strengthening of the safety property by an additional constraint that needs to be obeyed in any composition-invariant pair, where obtaining a composition-invariant pair is the target of the algorithm. This makes our algorithm *property directed*.

If an abstract state that satisfies $\varphi_{pre}(\mathcal{B})$ is added to *Unreach*, then Algorithm 1 determines that no solution exists (Line 9). Otherwise, it generates a new constraint for E based on the abstract state preceding $\hat{s}$ in the abstract counterexample (Line 12).

Constructing the Next Candidate Self Composition Function. Given the set of constraints in E and the formula *Unreach*, `Modify_SC` (Line 13) generates the next candidate composition function by (i) taking a constraint $(\hat{s}, M)$ such that $\hat{s} \not\models$ *Unreach* (typically the one that was added last), (ii) selecting a non-starving value M_{new} for $\hat{s}$ (such

[6] If the conditions $\{C_M\}_M$ defining f may overlap, we consider the condition C_M by which the transition from $\hat{s}_m$ to $\hat{s}_{m+1}$ was defined.

a value must exist, otherwise $\hat{s}$ would have been added to *Unreach*), and (iii) updating the conditions defining f' as follows:

$$C'_M = C_M \wedge \neg\hat{s}(\mathcal{P}) \qquad C'_{M_{\text{new}}} = (C_{M_{\text{new}}} \vee \hat{s}(\mathcal{P}))$$

The conditions of other values remain as before. This definition is facilitated by the fact that the same set of predicates is used both for defining f' and for defining the abstract states $\hat{s} \in \hat{S}$ (by which Inv is obtained). Note that in practice we do not explicitly turn f' to be undefined for $\gamma(\mathit{Unreach})$. However, these definitions are ignored. The definition ensures that f' is non-starving (satisfying condition **S3**) and that no two conditions $C'_{M_1} \neq C'_{M_2}$ overlap. While the latter is not required, it also does not restrict the generality of the approach (since the language we consider is closed under Boolean operations).

Theorem 2. *Let T be a transition system, $(pre, post)$ a k-safety property and $\mathcal{P}$ a set of predicates over $\mathcal{V}^{\|k}$. If Algorithm 1 returns "no solution" then there is no composition-invariant pair for T and $(pre, post)$ in $\mathcal{L}_\mathcal{P}$. Otherwise, $(f, Inv(\mathcal{P}))$ returned by Algorithm 1 is a composition-invariant pair in $\mathcal{L}_\mathcal{P}$, and thus $T \models^k (pre, post)$.*

Complexity. Each iteration of Algorithm 1 adds at least one constraint to E, excluding a potential value for f over some abstract state $\hat{s}$. An excluded values is never re-used. Hence, the number of iterations is at most the number of abstract states, $2^{|\mathcal{P}|}$, multiplied by the number of potential values for each abstract state, $n = 2^k$. Altogether, the number of iterations is at most $O(2^{|\mathcal{P}|} \cdot 2^k)$. Each iteration makes one call to `Abs_Reach` which checks reachability via predicate abstraction, hence, assuming that satisfiability checks in the original logic are at most exponential, its complexity is $2^{O(|\mathcal{P}|)}$. Therefore, the overall complexity of the algorithm is $2^{O(|\mathcal{P}|)+k}$. Typically, k is a small constant, hence the complexity is dominated by $2^{O(|\mathcal{P}|)}$.

5 Evaluation and Conclusion

Implementation. We implemented PDSC (Algorithm 1) in Python on top of Z3 [25]. Its input is a transition system encoded by Constrained Horn Clauses (CHC) in SMT2 format, a k-safety property and a set of predicates. The abstraction is implicitly encoded using the approach of [6], and is parameterized by a composition function that is modified in each iteration. For reachability checks (`Abs_Reach`) we use SPACER [22], which supports LRA and arrays. For the set of predicates used by PDSC, we implemented an automatic procedure that mines these predicates from the CHC. Additional predicates may be added manually.

Experiments. To evaluate PDSC, we compare it to SYNONYM [26], the current state of the art in k-safety verification.

To show the effectiveness of PDSC, we consider examples that require a *nontrivial* composition (these examples are detailed in [29]). We emphasize that the motivation for these example is originated in real-life scenarios. For example, Fig. 1 follows a pattern of constant-time execution. The results of these experiments are summarized in Table 1.

Table 1. Examples that require semantic compositions

Program	PDSC		SYNONYM
	Time(s)	Iteations	
DoubleSquareNI	7	33	fail
HalfSquareNI	3.4	28	fail
ArrayIntMod	58.2	168	fail
SquaresSum	2.8	4	fail
ArrayInsert	19.5	102	fail

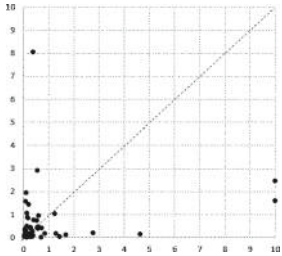

Fig. 2. Runtime comparison (in sec.): PDSC (x-axis) and SYNONYM (y-axis).

PDSC is able to find the right composition function and prove all of the examples, while SYNONYM cannot verify any of them. We emphasize that for these examples, lock-step composition is not sufficient. However, PDSC infers a composition that depends on the programs' state (variable values), rather than just program locations.

Next we consider Java programs from [26,30], which we manually converted to C, and then converted to CHC using SEAHORN [19]. For all but 3 examples, only 2 types of predicates, which we mined automatically, were sufficient for verification: (i) relational predicates derived from the pre- and post-conditions, and (ii) for simple loops that have an index variable (e.g., for iterating over an array), an equality predicate between the copies of the indices. These predicates were sufficient since we used a large-step encoding of the transition relation, hence the abstraction via predicates takes effect only at cut-points. For the remaining 3 examples, we manually added 2–4 predicates. With the exception of 1 example where a timeout of 10 seconds was reached, all examples were solved with a lock-step composition function. Yet, we include them to show that on examples with simple compositions PDSC performs similarly to SYNONYM. This can be seen in Fig. 2.

Conclusion and Future Work. This work formulates the problem of inferring a self composition function together with an inductive invariant for the composed program, thus capturing the interplay between the self composition and the difficulty of verifying the resulting composed program. To address this problem we present PDSC– an algorithm for inferring a semantic self composition, directed at verifying the composed program with a given language of predicates. We show that PDSC manages to find non-trivial self compositions that are beyond reach of existing tools. In future work, we are interested in further improving PDSC by extending it with additional (possibly lazy) predicate discovery abilities. This has the potential to both improve performance and verify properties over wider range of programs. Additionally, we consider exploring further generalization techniques during the inference procedure.

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Security-Aware Synthesis Using Delayed-Action Games

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Abstract. Stochastic multiplayer games (SMGs) have gained attention in the field of strategy synthesis for multi-agent reactive systems. However, standard SMGs are limited to modeling systems where all agents have full knowledge of the state of the game. In this paper, we introduce delayed-action games (DAGs) formalism that simulates hidden-information games (HIGs) as SMGs, where hidden information is captured by delaying a player's actions. The elimination of private variables enables the usage of SMG off-the-shelf model checkers to implement HIGs. Furthermore, we demonstrate how a DAG can be decomposed into subgames that can be independently explored, utilizing parallel computation to reduce the model checking time, while alleviating the state space explosion problem that SMGs are notorious for. In addition, we propose a DAG-based framework for strategy synthesis and analysis. Finally, we demonstrate applicability of the DAG-based synthesis framework on a case study of a human-on-the-loop unmanned-aerial vehicle system under stealthy attacks, where the proposed framework is used to formally model, analyze and synthesize security-aware strategies for the system.

1 Introduction

Stochastic multiplayer games (SMGs) are used to model reactive systems where nondeterministic decisions are made by multiple players [4,13,23]. SMGs extend probabilistic automata by assigning a player to each choice to be made in the game. This extension enables modeling of complex systems where the behavior of players is unknown at design time. The *strategy synthesis* problem aims to find a *winning strategy*, i.e., a strategy that guarantees that a set of objectives (or winning conditions) is satisfied [6,21]. Algorithms for synthesis include, for instance, value iteration and strategy iteration techniques, where multiple reward-based objectives are satisfied [2,9,17]. To tackle the state-space explosion problem, [29] presents an *assume-guarantee* synthesis framework that relies on synthesizing strategies on the component level first, before composing them into a global winning strategy. Mean-payoffs and ratio rewards are further investigated in [3]

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to synthesize ε-optimal strategies. Formal tools that support strategy synthesis via SMGs include PRISM-games [7,19] and Uppaal Stratego [10].

SMGs are classified based on the number of players that can make choices at each state. In *concurrent* games, more than one player is allowed to concurrently make choices at a given state. Conversely, *turn-based* games assign one player at most to each state. Another classification considers the information available to different players across the game [27]. *Complete-information* games (also known as *perfect-information* games [5]) grant all players complete access to the information within the game. In *symmetric* games, some information is equally hidden from all players. On the contrary, *asymmetric* games allow some players to have access to more information than the others [27].

This work is motivated by security-aware systems in which stealthy adversarial actions are potentially hidden from the system, where the latter can probabilistically and intermittently gain full knowledge about the current state. While hidden-information games (HIGs) can be used to model such systems by using private variables to capture hidden information [5], standard model checkers can only synthesize strategies for (full-information) SMGs; thus, demanding for alternative representations. The equivalence between turn-based semi-perfect information games and concurrent perfect-information games was shown [5]. Since a player's strategy mainly rely on full knowledge of the game state [9], using SMGs for synthesis produces strategies that may violate synthesis specifications in cases where required information is hidden from the player. *Partially-observable* stochastic games (POSGs) allow agents to have different belief states by incorporating uncertainty about both the current state and adversarial plans [15]. Techniques such as active sensing for online replanning [14] and grid-based abstractions of belief spaces [24] were proposed to mitigate synthesis complexity arising from partial observability. The notion of *delaying actions* has been studied as means for gaining information about a game to improve future strategies [18,30], but was not deployed as means for hiding information.

To this end, we introduce delayed-action games (DAGs)—a new class of games that simulate HIGs, where information is hidden from one player by delaying the actions of the others. The omission of private variables enables the use of off-the-shelf tools to implement and analyze DAG-based models. We show how DAGs (under some mild and practical assumptions) can be decomposed into subgames that can be independently explored, reducing the time required for synthesis by employing parallel computation. Moreover, we propose a DAG-based framework for strategy synthesis and analysis of security-aware systems. Finally, we demonstrate the framework's applicability through a case study of security-aware planning for an unmanned-aerial vehicle (UAV) system prone to stealthy cyber attacks, where we develop a DAG-based system model and further synthesize strategies with strong probabilistic security guarantees.

The paper is organized as follows. Section 2 presents SMGs, HIGs, and problem formulation. In Sect. 3, we introduce DAGs and show that they can simulate HIGs. Section 4 proposes a DAG-based synthesis framework, which we use for security-aware planning for UAVs in Sect. 5, before concluding the paper in Sect. 6.

2 Stochastic Games

In this section, we present turn-based stochastic games, which assume that all players have full information about the game state. We then introduce hidden-information games and their private-variable semantics.

Notation. We use $\mathbb{N}_0$ to denote the set of non-negative integers. $\mathcal{P}(A)$ denotes the powerset of A (i.e., 2^A). A variable v has a set of valuations $Ev\,(v)$, where $\eta\,(v) \in Ev\,(v)$ denotes one. We use Σ^* to denote the set of all finite words over alphabet Σ, including the empty word ϵ. The mapping $Eff : \Sigma^* \times Ev\,(v) \to Ev\,(v)$ indicates the effect of a finite word on $\eta\,(v)$. Finally, for general indexing, we use s_i or $s^{(i)}$, for $i \in \mathbb{N}_0$, while PL_γ denotes *Player* γ.

Turn-Based Stochastic Games (SMGs). SMGs can be used to model reactive systems that undergo both stochastic and nondeterministic transitions from one state to another. In a *turn-based* game,[1] actions can be taken at any state by at most one player. Formally, an SMG can be defined as follows [1,28,29].

Definition 1 (Turn-Based Stochastic Game). *A* turn-based game (SMG) *with players* $\Gamma = \{\text{I}, \text{II}, \bigcirc\}$ *is a tuple* $\mathcal{G} = \langle S, (S_\text{I}, S_\text{II}, S_\bigcirc), A, s_0, \delta \rangle$, *where*

- S *is a finite set of states, partitioned into* S_I, S_II *and* $S_\bigcirc$;
- $A = A_\text{I} \cup A_\text{II} \cup \{\tau\}$ *is a finite set of actions where* τ *is an empty action;*
- $s_0 \in S_\text{II}$ *is the initial state; and*
- $\delta : S \times A \times S \to [0, 1]$ *is a transition function, such that* $\delta(s, a, s') \in \{1, 0\}$, $\forall s \in S_\text{I} \cup S_\text{II}, a \in A$ *and* $s' \in S$, *and* $\delta(s, \tau, s') \in [0, 1]$, $\forall s \in S_\bigcirc$ *and* $s' \in S_\text{I} \cup S_\text{II}$, *where* $\sum_{s' \in S_\text{I} \cup S_\text{II}} \delta(s, \tau, s') = 1$ *holds.*

For all $s \in S_\text{I} \cup S_\text{II}$ and $a \in A_\text{I} \cup A_\text{II}$, we write $s \xrightarrow{a} s'$ if $\delta(s, a, s') = 1$. Similarly, for all $s \in S_\bigcirc$ we write $s \xrightarrow{p} s'$ if s' is randomly sampled with probability $p = \delta(s, \tau, s')$.

Hidden-Information Games. SMGs assume that all players have full knowledge of the current state, and hence provide *perfect-information* models [5]. In many applications, however, this assumption may not hold. A great example are security-aware models where stealthy adversarial actions can be hidden from the system; e.g., the system may not even be aware that it is under attack. On the other hand, *hidden-information* games (HIGs) refer to games where one player does not have complete access to (or knowledge of) the current state. The notion of hidden information can be formalized with the use of *private variables* (PVs) [5]. Specifically, a game state can be encoded using variables $v_\mathcal{T}$ and $v_\mathcal{B}$, representing the true information, which is only known to PL_I, and PL_II belief, respectively.

[1] The term *turn-based* indicates that at any state only one player can play an action. It does not necessarily imply that players take fair turns.

Definition 2 (Hidden-Information Game). *A* hidden-information stochastic game (HIG) *with players* $\Gamma = \{\mathrm{I}, \mathrm{II}, \bigcirc\}$ *over a set of variables* $V = \{v_{\mathcal{T}}, v_{\mathcal{B}}\}$ *is a tuple* $\mathcal{G}_{\mathsf{H}} = \langle S, (S_{\mathrm{I}}, S_{\mathrm{II}}, S_{\bigcirc}), A, s_0, \beta, \delta \rangle$, *where*

- *set of states* $S \subseteq Ev\,(v_{\mathcal{T}}) \times Ev\,(v_{\mathcal{B}}) \times \mathcal{P}\,(Ev\,(v_{\mathcal{T}})) \times \Gamma$, *partitioned in* $S_{\mathrm{I}}, S_{\mathrm{II}}, S_{\bigcirc}$;
- $A = A_{\mathrm{I}} \cup A_{\mathrm{II}} \cup \{\tau, \theta\}$ *is a finite set of actions, where* τ *denotes an empty action, and* θ *is the action capturing* PL_{II} *attempt to reveal the true value* $v_{\mathcal{T}}$;
- $s_0 \in S_{\mathrm{II}}$ *is the initial state;*
- $\beta\colon A_{\mathrm{II}} \to \mathcal{P}(A_I)$ *is a function that defines the set of available* PL_{I} *actions, based on* PL_{II} *action; and*
- $\delta\colon S \times A \times S \to [0,1]$ *is a transition function such that* $\delta(s_{\mathrm{I}}, a, s_{\bigcirc}) = \delta(s_{\bigcirc}, a, s_{\mathrm{I}}) = 0$, *and* $\delta(s_{\mathrm{II}}, \theta, s_{\bigcirc})$, $\delta(s_{\mathrm{II}}, a, s_{\mathrm{I}})$, $\delta(s_{\mathrm{I}}, a, s_{\mathrm{II}}) \in \{0,1\}$ *for all* $s_{\mathrm{I}} \in S_{\mathrm{I}}$, $s_{\mathrm{II}} \in S_{\mathrm{II}}$, $s_{\bigcirc} \in S_{\bigcirc}$ *and* $a \in A$, *where* $\sum_{s' \in S_{\mathrm{II}}} \delta(s_{\bigcirc}, \tau, s') = 1$.

In the above definition, δ only allows transitions s_{I} to s_{II}, s_{II} to s_{I} or $s_{\bigcirc}$, with s_{II} to $s_{\bigcirc}$ conditioned by action θ, and probabilistic transitions $s_{\bigcirc}$ to s_{II}. A game state can be written as $s = (t, u, \Omega, \gamma)$, but to simplify notation we use $s_{\gamma}\,(t, u, \Omega)$ instead, where $t \in Ev\,(v_{\mathcal{T}})$ is the *true* value of the game, $u \in Ev\,(v_{\mathcal{B}})$ is $\mathrm{PL}_{\mathrm{II}}$ current *belief*, $\Omega \in \mathcal{P}(Ev\,(v_{\mathcal{T}})) \setminus \{\emptyset\}$ is $\mathrm{PL}_{\mathrm{II}}$ *belief space*, and $\gamma \in \Gamma$ is the current player's index. When the truth is hidden from $\mathrm{PL}_{\mathrm{II}}$, the belief space Ω is the *information set* [27], capturing $\mathrm{PL}_{\mathrm{II}}$ knowledge about the possible true values.

Example 1 (Belief vs. True Value). Our motivating example is a system that consists of a UAV and a human operator. For localization, the UAV mainly relies on a GPS sensor that can be compromised to effectively steer the UAV away from its original path. While aggressive attacks can be detected, some may remain stealthy by introducing only bounded errors at each step [16,20,22,26]. For example, Fig. 1 shows a UAV ($\mathrm{PL}_{\mathrm{II}}$) occupying zone A and flying north (N). An adversary (PL_{I}) can launch a stealthy attack targeting its GPS, introducing a bounded error (NE, NW) to remain stealthy. The set of stealthy actions available to the attacker depends on the preceding UAV action, which is captured by the function β, where $\beta(\mathsf{N}) = \{\mathsf{NE}, \mathsf{N}, \mathsf{NW}\}$. Being unaware of the attack, the UAV believes that it is entering zone C, while the true new location is D due to the attack (NE). Initially, $\eta\,(v_{\mathcal{T}}) = \eta\,(v_{\mathcal{B}}) = z_A$, and $\Omega = \{z_A\}$ as the UAV is certain it is in zone z_A. In s_2, $\eta\,(v_{\mathcal{B}}) = z_C$, yet $\eta\,(v_{\mathcal{T}}) = z_D$. Although $v_{\mathcal{T}}$ is hidden, $\mathrm{PL}_{\mathrm{II}}$ is aware that $\eta\,(v_{\mathcal{T}})$ is in $\Omega = \{z_B, z_C, z_D\}$.

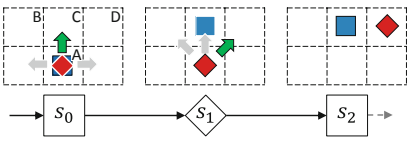


Fig. 1. The UAV belief (solid square) vs. the true value (solid diamond) of its location.

HIG Semantics. $\mathcal{G}_{\mathsf{H}}$ semantics is described using the rules shown in Fig. 2, where H2 and H3 capture $\mathrm{PL}_{\mathrm{II}}$ and PL_{I} moves, respectively. The rule H4 specifies that a $\mathrm{PL}_{\mathrm{II}}$ attempt θ to reveal the true value can succeed with probability p_i where $\mathrm{PL}_{\mathrm{II}}$ belief is updated (i.e., $u' = t$), and remains unchanged otherwise.

$$
\begin{aligned}
&\textsf{H1}\colon\ s_0 = s_{\text{II}}(t_0, u_0, \Omega_0) && \text{if } t_0 = u_0,\ \Omega_0 = \{t_0\}\\
&\textsf{H2}\colon\ s_{\text{II}}(t,u,\Omega) \xrightarrow{a_i} s_{\text{I}}(t',u',\Omega') && \text{if } a_i \in A_{\text{II}},\ t'=t,\ u'=\mathit{Eff}(a_i,u),\\
& && \quad \Omega' = \{t' \mid t' = \mathit{Eff}(b_i,t)\ \forall b_i \in \beta(a_i), t \in \Omega\}\\
&\qquad\quad \xrightarrow{\theta} s_{\bigcirc}(t',u',\Omega') && \text{if } t'=t,\ u'=u,\ \Omega'=\Omega\\
&\textsf{H3}\colon\ s_{\text{I}}(t,u,\Omega) \xrightarrow{b_i} s_{\text{II}}(t',u',\Omega') && \text{if } b_i \in \beta(a_i),\ t'=\mathit{Eff}(b_i,t),\ u'=u,\ \Omega'=\Omega\\
&\textsf{H4}\colon\ s_{\bigcirc}(t,u,\Omega) \xrightarrow{p_i} s_{\text{II}}(t',u',\Omega') && \text{if } t'=t,\ u'=t,\ \Omega'=\{t\},\ p_i=\delta(s_{\bigcirc},\tau,s_{\text{II}})\\
&\qquad\quad \xrightarrow{1-p_i} s_{\text{II}}(t',u',\Omega') && \text{if } t'=t,\ u'=u,\ \Omega'=\Omega,\ 1-p_i=\delta(s_{\bigcirc},\tau,s_{\text{II}})
\end{aligned}
$$

Fig. 2. Semantic rules for an HIG.

Example 2 (HIG Semantics). Continuing Example 1, let us assume that the set of actions $A_{\text{I}} = A_{\text{II}} = \{\mathsf{N}, \mathsf{S}, \mathsf{E}, \mathsf{W}, \mathsf{NE}, \mathsf{NW}, \mathsf{SE}, \mathsf{SW}\}$, and that $\theta = \mathsf{GT}$ is a geolocation task that attempts to reveal the true value of the game.[2] Now, consider the scenario illustrated in Fig. 3. At the initial state s_0, the UAV attempts to move north (N), progressing the game to the state s_1, where the adversary takes her turn by selecting an action from the set $\beta(\mathsf{N}) = \{\mathsf{NE}, \mathsf{N}, \mathsf{NW}\}$. The players take turns until the UAV performs a geolocation task GT, moving from the state s_4 to s_5. With probability $p = \delta(s_5, \tau, s_6)$, the UAV detects its true location and updates its belief accordingly (i.e., to s_6). Otherwise, the belief remains the same (i.e., equal to s_4).

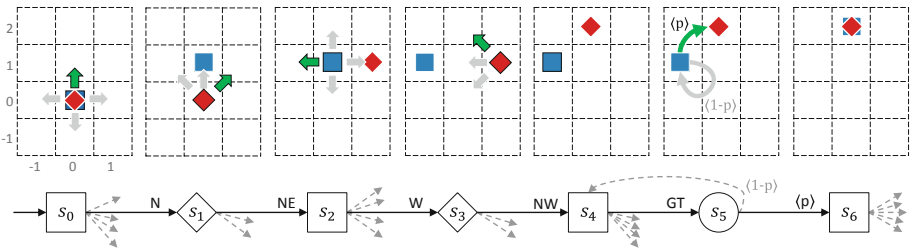


Fig. 3. An example of the UAV motion in a 2D-grid map, modeled as an HIG. Solid squares represent the UAV belief, while solid diamonds represent the ground truth. The UAV action GT denotes performing a geolocation task.

Problem Formulation. Following the system described in Example 2, we now consider the composed HIG $\mathcal{G}_{\mathsf{H}} = \mathcal{M}_{\text{adv}} \| \mathcal{M}_{\text{uav}} \| \mathcal{M}_{\text{as}}$ shown in Fig. 4; the HIG-based model incorporates standard models of a UAV ($\mathcal{M}_{\text{uav}}$), an adversary ($\mathcal{M}_{\text{adv}}$), and a geolocation-task advisory system ($\mathcal{M}_{\text{as}}$) (e.g., as introduced in [11,12]). Here, the probability of a successful detection $p(v_{\mathcal{T}}, v_{\mathcal{B}})$ is a function of both the location the UAV believes to be its current location ($v_{\mathcal{B}}$) as well

[2] A geolocation task is an attempt to localize the UAV by examining its camera feed.

as the ground truth location that the UAV actually occupies ($v_{\mathcal{T}}$). Reasoning about the flight plan using such model becomes problematic since the ground truth $v_{\mathcal{T}}$ is inherently unknown to the UAV (i.e., PL_{II}), and thus so is $p(v_{\mathcal{T}}, v_{\mathcal{B}})$. Furthermore, such representation, where some information is hidden, is not supported by off-the-shelf SMG model checkers. Consequently, for such HIGs, *our goal is to find an alternative representation that is suitable for strategy synthesis using off-the-shelf SMG model-checkers.*

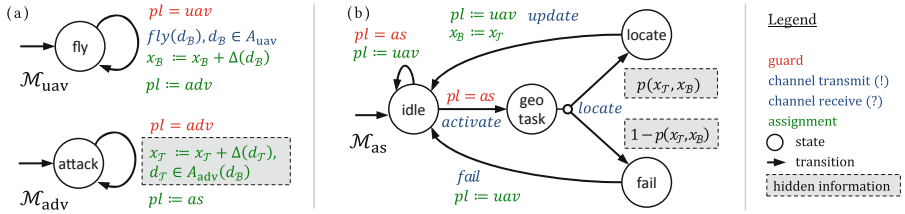


Fig. 4. An example of an HIG-based system model comprised of the UAV ($\mathcal{M}_{\text{uav}}$), the adversary ($\mathcal{M}_{\text{adv}}$), and the AS ($\mathcal{M}_{\text{as}}$). Framed information is hidden from the UAV-AS.

3 Delayed-Action Games

In this section, we provide an alternative representation of HIGs that eliminates the use of private variables—we introduce Delayed-Action Games (DAGs) that exploit the notion of *delayed actions*. Furthermore, we show that for any HIG, a DAG that simulates the former can be constructed.

Delayed Actions. Informally, a DAG reconstructs an HIG such that actions of PL_{I} (the player with access to perfect information) follow the actions of PL_{II}, i.e., PL_{I} actions are *delayed*. This rearrangement of the players' actions provides a means to hide information from PL_{II} without the use of private variables, since in this case, at PL_{II} states, PL_{I} actions have not occurred yet. In this way, PL_{II} can act as though she has complete information at the moment she makes her decision, as the future state has not yet happened and so cannot be known. In essence, the formalism can be seen as a partial ordering of the players' actions, exploiting the (partial) superposition property that a wide class of physical systems exhibit. To demonstrate this notion, let us consider DAG modeling on our running example.

Example 3 (Delaying Actions). Figure 5 depicts the (HIG-based) scenario from Fig. 3, but in the corresponding DAG, where the UAV actions are performed first (in $\hat{s}_0, \hat{s}_1, \hat{s}_2$), followed by the adversary delayed actions (in $\hat{s}_3, \hat{s}_4$). Note that, in the DAG model, at the time the UAV executed its actions ($\hat{s}_0, \hat{s}_1, \hat{s}_2$) the adversary actions had not occurred (yet). Moreover, $\hat{s}_0$ and $\hat{s}_6$ (Fig. 5) share the same belief and true values as s_0 and s_6 (Fig. 3), respectively, though the transient states do not exactly match. This will be used to show the relationship between the games.

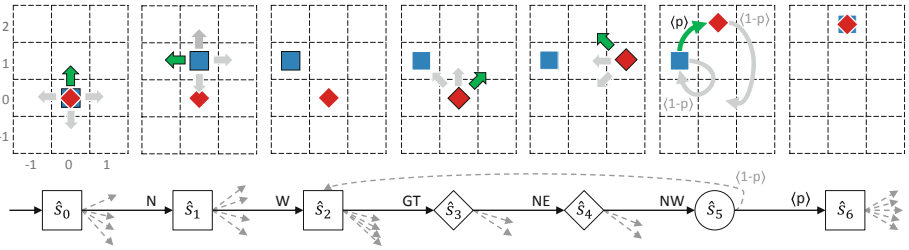


Fig. 5. The same scenario as in Fig. 3, modeled as a DAG. Solid squares represent UAV belief, while solid diamonds represent the ground truth. The UAV action GT denotes performing a geolocation task.

The advantage of this approach is twofold. First, the elimination of private variables enables simulation of an HIG using a full-information game. Thus, the formulation of the strategy synthesis problem using off-the-shelf SMG-based tools becomes feasible. In particular, a $\mathrm{PL_{II}}$ synthesized strategy becomes dependent on the knowledge of $\mathrm{PL_I}$ behavior (possible actions), rather than the specific (hidden) actions. We formalize a DAG as follows.

Definition 3 (Delayed-Action Game). *A* DAG *of an HIG* $\mathcal{G}_{\mathsf{H}} = \langle S, (S_{\mathrm{I}}, S_{\mathrm{II}}, S_{\bigcirc}), A, s_0, \beta, \delta \rangle$*, with players* $\Gamma = \{\mathrm{I}, \mathrm{II}, \bigcirc\}$ *over a set of variables* $V = \{v_{\mathcal{T}}, v_{\mathcal{B}}\}$ *is a tuple* $\mathcal{G}_{\mathsf{D}} = \langle \hat{S}, (\hat{S}_{\mathrm{I}}, \hat{S}_{\mathrm{II}}, \hat{S}_{\bigcirc}), A, \hat{s}_0, \beta, \hat{\delta} \rangle$ *where*

- $\hat{S} \subseteq Ev\,(v_{\mathcal{T}}) \times Ev\,(v_{\mathcal{B}}) \times A^*_{\mathrm{II}} \times \mathbb{N}_0 \times \Gamma$ *is the set of states, partitioned into* $\hat{S}_{\mathrm{I}}, \hat{S}_{\mathrm{II}}$ *and* $\hat{S}_{\bigcirc}$*;*
- $\hat{s}_0 \in \hat{S}_{\mathrm{II}}$ *is the initial state; and*
- $\hat{\delta}\colon \hat{S} \times A \times \hat{S} \to [0,1]$ *is a transition function such that* $\hat{\delta}(\hat{s}_{\mathrm{II}}, a, \hat{s}_{\bigcirc}) = \hat{\delta}(\hat{s}_{\mathrm{I}}, a, \hat{s}_{\mathrm{II}}) = \hat{\delta}(\hat{s}_{\bigcirc}, a, \hat{s}_{\mathrm{I}}) = 0$*, and* $\hat{\delta}(\hat{s}_{\mathrm{II}}, a, \hat{s}_{\mathrm{II}}) \in \{0,1\}$*,* $\hat{\delta}(\hat{s}_{\mathrm{II}}, \theta, \hat{s}_{\mathrm{I}}) \in \{0,1\}$*,* $\hat{\delta}(\hat{s}_{\mathrm{I}}, a, \hat{s}_{\mathrm{I}}) \in \{0,1\}$*,* $\hat{\delta}(\hat{s}_{\mathrm{I}}, a, \hat{s}_{\bigcirc}) \in \{0,1\}$*, for all* $\hat{s}_{\mathrm{I}} \in \hat{S}_{\mathrm{I}}$*,* $\hat{s}_{\mathrm{II}} \in \hat{S}_{\mathrm{II}}$*,* $\hat{s}_{\bigcirc} \in \hat{S}_{\bigcirc}$ *and* $a \in A$*, where* $\sum_{\hat{s}' \in \hat{S}_{\mathrm{II}}} \delta(\hat{s}_{\bigcirc}, a, \hat{s}') = 1$*.*

Note that, in contrast to transition function δ in HIG $\mathcal{G}_{\mathsf{H}}$, $\hat{\delta}$ in DAG $\mathcal{G}_{\mathsf{D}}$ only allows transitions $\hat{s}_{\mathrm{II}}$ to $\hat{s}_{\mathrm{II}}$ or $\hat{s}_{\mathrm{I}}$, as well as $\hat{s}_{\mathrm{I}}$ to $\hat{s}_{\mathrm{I}}$ or $\hat{s}_{\bigcirc}$, and probabilistic transitions $\hat{s}_{\bigcirc}$ to $\hat{s}_{\mathrm{II}}$; also note that $\hat{s}_{\mathrm{II}}$ to $\hat{s}_{\mathrm{I}}$ is conditioned by the action θ.

DAG Semantics. A DAG state is a tuple $\hat{s} = (\hat{t}, \hat{u}, w, j, \gamma)$, which for simplicity we shorthand as $\hat{s}_{\gamma}\,(\hat{t}, \hat{u}, w, j)$, where $\hat{t} \in Ev\,(v_{\mathcal{T}})$ is the last known true value, $\hat{u} \in Ev\,(v_{\mathcal{B}})$ is $\mathrm{PL_{II}}$ belief, $w \in A^*_{\mathrm{II}}$ captures $\mathrm{PL_{II}}$ actions taken since the last known true value, $j \in \mathbb{N}_0$ is an index on w, and $\gamma \in \Gamma$ is the current player index. The game transitions are defined using the semantic rules from Fig. 6. Note that $\mathrm{PL_{II}}$ can execute multiple moves (i.e., actions) before executing θ to attempt to reveal the true value (D2), moving to a $\mathrm{PL_I}$ state where $\mathrm{PL_I}$ executes all her delayed actions before reaching a 'revealing' state $\hat{s}_{\bigcirc}$ (D3). Finally, the revealing attempt can succeed with probability p_i where $\mathrm{PL_{II}}$ belief is updated (i.e., $\hat{u}' = \hat{t}$), or otherwise remains unchanged (D4).

$$
\begin{aligned}
&\mathsf{D1}\colon \hat{s}_0 = \hat{s}_{\mathrm{II}}(\hat{t}_0, \hat{u}_0, w_0, 0) && \text{if } \hat{t}_0 = \hat{u}_0,\ w_0 = \epsilon \\
&\mathsf{D2}\colon \hat{s}_{\mathrm{II}}\left(\hat{t}, \hat{u}, w, 0\right) \xrightarrow{a_i} \hat{s}_{\mathrm{II}}\left(\hat{t}', \hat{u}', w', 0\right) && \text{if } a_i \in A_{\mathrm{II}},\ \hat{t}' = \hat{t},\ \hat{u}' = \mathit{Eff}(a_i, \hat{u}),\ w' = wa_i \\
&\qquad \xrightarrow{\theta} \hat{s}_{\mathrm{I}}\left(\hat{t}', \hat{u}', w', 0\right) && \text{if } \hat{t}' = \hat{t},\ \hat{u}' = \hat{u},\ w' = w \\
&\mathsf{D3}\colon \hat{s}_{\mathrm{I}}\left(\hat{t}, \hat{u}, w, j\right) \xrightarrow{b_i} \hat{s}_{\mathrm{I}}\left(\hat{t}', \hat{u}', w', j{+}1\right) && \text{if } b_i \in \beta(w_j),\ \hat{t}' = \mathit{Eff}\left(b_i, \hat{t}\right),\ \hat{u}' = \hat{u},\ w' = w,\ j < |w| - 1 \\
&\qquad \xrightarrow{b_i} \hat{s}_{\bigcirc}\left(\hat{t}', \hat{u}', w', j\right) && \text{if } b_i \in \beta(w_j),\ \hat{t}' = \mathit{Eff}\left(b_i, \hat{t}\right),\ \hat{u}' = \hat{u},\ w' = w,\ j = |w| - 1 \\
&\mathsf{D4}\colon \hat{s}_{\bigcirc}\left(\hat{t}, \hat{u}, w, j\right) \xrightarrow{p_i} \hat{s}_{\mathrm{II}}\left(\hat{t}', \hat{u}', w', 0\right) && \text{if } \hat{t}' = \hat{t},\ \hat{u}' = \hat{t},\ w' = \epsilon,\ p_i = \hat{\delta}(\hat{s}_{\bigcirc}, \hat{s}_{\mathrm{II}}) \\
&\qquad \xrightarrow{1-p_i} \hat{s}_{\mathrm{II}}\left(\hat{t}', \hat{u}', w', 0\right) && \text{if } \hat{t}' = \hat{t}_0,\ \hat{u}' = \hat{u},\ w' = w,\ q_i = \hat{\delta}(\hat{s}_{\bigcirc}, \hat{s}_{\mathrm{II}})
\end{aligned}
$$

Fig. 6. Semantic rules for DAGs.

In both $\mathcal{G}_{\mathsf{H}}$ and $\mathcal{G}_{\mathsf{D}}$, we label states where all players have full knowledge of the current state as *proper*. We also say that two states are similar if they agree on the belief, and equivalent if they agree on both the belief and ground truth.

Definition 4 (States). *Let $s_\gamma(t, u, \Omega) \in S$ and $\hat{s}_{\hat{\gamma}}(\hat{t}, \hat{u}, w, j) \in \hat{S}$. We say:*

- *s_γ is* proper *iff $\Omega = \{t\}$, denoted by $s_\gamma \in \mathrm{Prop}(\mathcal{G}_{\mathsf{H}})$.*
- *$\hat{s}_{\hat{\gamma}}$ is* proper *iff $w = \epsilon$, denoted by $\hat{s}_{\hat{\gamma}} \in \mathrm{Prop}(\mathcal{G}_{\mathsf{D}})$.*
- *s_γ and $\hat{s}_{\hat{\gamma}}$ are* similar *iff $\hat{u} = u$, $\hat{t} \in \Omega$, and $\gamma = \hat{\gamma}$, denoted by $s_\gamma \sim \hat{s}_{\hat{\gamma}}$.*
- *s_γ, $\hat{s}_{\hat{\gamma}}$ are* equivalent *iff $t = \hat{t}$, $u = \hat{u}$, $w = \epsilon$, and $\gamma = \hat{\gamma}$, denoted by $s_\gamma \simeq \hat{s}_{\hat{\gamma}}$.*

From the above definition, we have that $s \simeq \hat{s} \implies s \in \mathrm{Prop}(\mathcal{G}_{\mathsf{H}}), \hat{s} \in \mathrm{Prop}(\mathcal{G}_{\mathsf{D}})$. We now define *execution fragments*, possible progressions from a state to another.

Definition 5 (Execution Fragment). *An* execution fragment *(of either an SMG, DAG or HIG) is a finite sequence of states, actions and probabilities $\varrho = s_0 a_1 p_1 s_1 a_2 p_2 s_2 \ldots a_n p_n s_n$ such that $(s_i \xrightarrow{a_{i+1}} s_{i+1}) \vee (s_i \xrightarrow{\langle p_{i+1} \rangle} s_{i+1}), \forall i \geq 0$.*[3]

We use *first*(ϱ) and *last*(ϱ) to refer to the first and last states of ϱ, respectively. If both states are proper, we say that ϱ is *proper* as well, denoted by $\varrho \in \mathrm{Prop}(\mathcal{G}_{\mathsf{H}})$.[4] Moreover, ϱ is *deterministic* if no probabilities appear in the sequence.

Definition 6 (Move). *A* move *m_γ of an execution ϱ from state $s \in \varrho$, denoted by $move_\gamma(s, \varrho)$, is a sequence of actions $a_1 a_2 \ldots a_i \in A_\gamma^*$ that player γ performs in ϱ starting from s.*

By omitting the player index we refer to the moves of all players. To simplify notation, we use $move(\varrho)$ as a short notation for $move(first(\varrho), \varrho)$. We write $(m)(first(\varrho)) = last(\varrho)$ to denote that the execution of move m from the $first(\varrho)$ leads to the $last(\varrho)$. This allows us to now define the *delay operator* as follows.

[3] For deterministic transitions, $p = 1$, hence omitted from ϱ for readability.

[4] An execution fragment lives in the transition system (TS), i.e., $\varrho \in \mathrm{Prop}(\mathrm{TS}(\mathcal{G}))$. We omit TS for readability.

Definition 7 (Delay Operator). *For an $\mathcal{G}_{\mathsf{H}}$, let $m = move(\varrho) = a_1 b_1 \dots a_n b_n \theta$ be a move for some deterministic $\varrho \in \mathrm{TS}(\mathcal{G}_{\mathsf{H}})$, where $a_1 ... a_n \in A_{\mathrm{II}}^*, b_1 ... b_n \in A_{\mathrm{I}}^*$. The delay operator, denoted by $\overline{m}$, is defined by the rule $\overline{m} = a_1 \dots a_n \theta b_1 \dots b_n$.*

Intuitively, the delay operator shifts $\mathrm{PL_I}$ actions to the right of $\mathrm{PL_{II}}$ actions up until the next probabilistic state. For example,

$$
\begin{array}{rlccccccccccccc}
\text{if} & \rho = & s_{\mathrm{II}}^{(0)} & \xrightarrow{a_1} & s_{\mathrm{I}}^{(1)} & \xrightarrow{b_2} & s_{\mathrm{II}}^{(2)} & \xrightarrow{\theta} & s_{\bigcirc}^{(3)} & \xrightarrow{p_3} & s_{\mathrm{II}}^{(4)} & \xrightarrow{a_4} & s_{\mathrm{I}}^{(5)} & \xrightarrow{b_5} & s_{\mathrm{II}}^{(6)} & \xrightarrow{a_6} & s_{\mathrm{I}}^{(7)} & \xrightarrow{b_7} & s_{\mathrm{II}}^{(8)} \\
\text{then} & m = & & a_1 & & b_2 & & \theta & & \tau & & a_4 & & b_5 & & a_6 & & b_7, & \\
\text{and} & \overline{m} = & & a_1 & & \theta & & b_2 & & \tau & & a_4 & & a_6 & & b_5 & & b_7. &
\end{array}
$$

Simulation Relation. Given an HIG $\mathcal{G}_{\mathsf{H}}$, we first define the corresponding DAG $\mathcal{G}_{\mathsf{D}}$.

Definition 8 (Correspondence). *Given an HIG $\mathcal{G}_{\mathsf{H}}$, a corresponding DAG $\mathcal{G}_{\mathsf{D}} = \mathfrak{D}[\mathcal{G}_{\mathsf{H}}]$ is a DAG that follows the semantic rules displayed in Fig. 7.*

$$
\begin{array}{lcl}
s_0 = s_{\mathrm{II}}(t_0, u_0, \Omega_0) & \Longrightarrow & \hat{s}_0 = \hat{s}_{\mathrm{II}}(\hat{t}_0, \hat{u}_0, w_0, 0) \text{ s.t. } \hat{t}_0 = t_0,\ \hat{u}_0 = u_0 \\
s_{\mathrm{II}}(t, u, \Omega) \xrightarrow{a_i} s_{\mathrm{I}}(t', u', \Omega') & \Longrightarrow & \hat{s}_{\mathrm{II}}\left(\hat{t}, \hat{u}, w, 0\right) \xrightarrow{a_i} \hat{s}_{\mathrm{II}}\left(\hat{t}', \hat{u}', w', 0\right) \text{ s.t. } \hat{u} = u \\
s_{\mathrm{II}}(t, u, \Omega) \xrightarrow{\theta_i} s_{\bigcirc}(t', u', \Omega') & \Longrightarrow & \hat{s}_{\mathrm{II}}\left(\hat{t}, \hat{u}, w, 0\right) \xrightarrow{\theta_i} s_{\mathrm{I}}\left(\hat{t}', \hat{u}', w', 0\right) \text{ s.t. } \hat{u} = u \\
s_{\mathrm{I}}(t, u, \Omega) \xrightarrow{b_i} s_{\mathrm{II}}(t', u', \Omega') & \Longrightarrow & \hat{s}_{\mathrm{I}}\left(\hat{t}, \hat{u}, w, j\right) \xrightarrow{b_i} s_{\mathrm{I}}\left(\hat{t}', \hat{u}', w', j{+}1\right) \text{ s.t. } \hat{t} = t, j < |w| \\
s_{\mathrm{I}}(t, u, \Omega) \xrightarrow{b_i} s_{\mathrm{II}}(t', u', \Omega') & \Longrightarrow & \hat{s}_{\mathrm{I}}\left(\hat{t}, \hat{u}, w, j\right) \xrightarrow{b_i} s_{\bigcirc}\left(\hat{t}', \hat{u}', w', j\right) \text{ s.t. } \hat{t} = t, j = |w| \\
s_{\bigcirc}(t, u, \Omega) \xrightarrow{p_i} s_{\mathrm{II}}(t', u', \Omega') & \Longrightarrow & \hat{s}_{\bigcirc}\left(\hat{t}, \hat{u}, w, j\right) \xrightarrow{p_i} \hat{s}_{\mathrm{II}}\left(\hat{t}', \hat{u}', w', 0\right) \text{ s.t. } \hat{t} = t,\ \hat{u} = u \\
s_{\bigcirc}(t, u, \Omega) \xrightarrow{1-p_i} s_{\mathrm{II}}(t', u', \Omega') & \Longrightarrow & \hat{s}_{\bigcirc}\left(\hat{t}, \hat{u}, w, j\right) \xrightarrow{1-p_i} \hat{s}_{\mathrm{II}}\left(\hat{t}', \hat{u}', w', 0\right) \text{ s.t. } \hat{t} = t,\ \hat{u} = u
\end{array}
$$

Fig. 7. Semantic rules for HIG-to-DAG transformation.

For the rest of this section, we consider $\mathcal{G}_{\mathsf{D}} = \mathfrak{D}[\mathcal{G}_{\mathsf{H}}]$, and use $\varrho \in \mathrm{TS}(\mathcal{G}_{\mathsf{H}})$ and $\hat{\varrho} \in \mathrm{TS}(\mathcal{G}_{\mathsf{D}})$ to denote two execution fragments of the HIG and DAG, respectively. We say that ϱ and $\hat{\varrho}$ are *similar*, denoted by $\varrho \sim \hat{\varrho}$, iff $first(\varrho) \simeq first(\hat{\varrho})$, $last(\varrho) \sim last(\hat{\varrho})$, and $\overline{move(\varrho)} = move(\hat{\varrho})$.

Definition 9 (Game Proper Simulation). *A game $\mathcal{G}_{\mathsf{D}}$ properly simulates $\mathcal{G}_{\mathsf{H}}$, denoted by $\mathcal{G}_{\mathsf{D}} \rightsquigarrow \mathcal{G}_{\mathsf{H}}$, iff $\forall \varrho \in \mathrm{Prop}(\mathcal{G}_{\mathsf{H}})$, $\exists \hat{\varrho} \in \mathrm{Prop}(\mathcal{G}_{\mathsf{D}})$ such that $\varrho \sim \hat{\varrho}$.*

Before proving the existence of the simulation relation, we first show that if a move is executed on two equivalent states, then the terminal states are similar.

Lemma 1 (Terminal States Similarity). *For any $s_0 \simeq \hat{s}_0$ and a deterministic $\varrho \in \mathrm{TS}(\mathcal{G}_{\mathsf{H}})$ where $first(\varrho) = s_0$, $last(\varrho) \in S_{\mathrm{II}}$, then $last(\varrho) \sim \left(\overline{move(\varrho)}\right)(\hat{s}_0)$ holds.*

Proof. Let $last(\varrho_i) = s^{(i)}_{\gamma_i}(t_i, u_i, \Omega_i)$ and $\left(\overline{move(\varrho_i)}\right)(\hat{s}_0) = \hat{s}^{(i)}_{\hat{\gamma}_i}(\hat{t}_i, \hat{u}_i, w_i, j_i)$, where $move(\varrho_i) = a_1 b_1 ... a_i b_i \theta$. We then write $\overline{move(\varrho)} = a_1 ... a_i \theta b_1 ... b_i$. We use induction over i as follows:

- Base ($i=0$): $\varrho_0 = s_0 \implies s^{(0)} \simeq \hat{s}^{(0)}$ where $u_0 = \hat{u}_0$ and $t_0 = \hat{t}_0$.
- Induction ($i > 0$): Assume that the claim holds for $move(\varrho_{i-1}) = a_1 b_1 ... a_{i-1} b_{i-1} \theta$, i.e., $u_{i-1} = \hat{u}_{i-1}$ and $\hat{t}_{i-1} \in \Omega_{i-1}$. For ϱ_i we have that $u_i = \mathit{Eff}(a_i, u_{i-1})$ and $\hat{u}_i = \mathit{Eff}(a_i, \hat{u}_{i-1})$. Also, $t_i = \mathit{Eff}(b_i, t_{i-1}) \in \Omega_i$ and $\hat{t}_i = \mathit{Eff}(b_i, \hat{t}_{i-1})$. Hence, $u_i = \hat{u}_i$, $\hat{t}_i \in \Omega_i$ and $\hat{\gamma}_i = \gamma_i = \bigcirc$. Thus, $s^{(i)} \sim \hat{s}^{(i)}$ holds. The same can be shown for $move(\varrho) = a_1 b_1 ... a_i b_i$ where no θ occurs. □

Theorem 1 (Probabilistic Simulation). *For any $s_0 \simeq \hat{s}_0$ and $\varrho \in \mathrm{Prop}(\mathcal{G}_\mathsf{H})$ where $first(\varrho) = s_0$, it holds that*

$$\Pr\left[last(\varrho) = s'\right] = \Pr\left[\left(\overline{move(\varrho)}\right)(\hat{s}_0) = \hat{s}'\right] \quad \forall s', \hat{s}' \;\; s.t. \;\; s' \simeq \hat{s}'.$$

Proof. We can rewrite ϱ as $\varrho = \varrho_0 \xrightarrow{p_1} \varrho_1 \cdots \varrho_{n-1} \xrightarrow{p_n} s^{(n)}_{\mathrm{II}}$, where $\varrho_0, \varrho_1, \ldots, \varrho_{n-1}$ are deterministic. Let $first(\varrho_i) = s^{(i)}_{\mathrm{II}}(t_i, u_i, \Omega_i)$, $last(\varrho_i) = s^{(i)}_{\bigcirc}(t'_i, u'_i, \Omega'_i)$, and $\left(\overline{move(\varrho)}\right)(\hat{s}_0) = \hat{s}^{(n)}(\hat{t}_n, \hat{u}_n, w_n, j_n)$. We use induction over n as follows:

- Base ($n=0$): for ϱ to be deterministic and proper, $\varrho = \varrho_0 = s^{(0)}$ holds.
- Case ($n = 1$): $p_1 = p(t'_0, u'_0)$. From Lemma 1, $\hat{u}_1 = u_1$ and $\hat{t}_1 = t_1$. Hence, $\Pr\left[last(\varrho) = s^{(1)}_{\mathrm{II}}\right] = \Pr\left[\left(\overline{move(\varrho)}\right)(\hat{s}_0) = \hat{s}^{(1)}_{\mathrm{II}}\right] = p(t'_0, u'_0)$ and $s^{(1)}_{\mathrm{II}} \simeq \hat{s}^{(1)}_{\mathrm{II}}$.
- Induction ($n > 1$): It is straightforward to infer that $p_n = p\left(t'_{n-1}, u'_{n-1}\right)$, hence $\Pr\left[last(\varrho) = s^{(n)}_{\mathrm{II}}\right] = \Pr\left[\left(\overline{move(\varrho)}\right)\left(\hat{s}^{(0)}\right) = \hat{s}^{(n)}\right] = P$, and $s^{(n)}_{\mathrm{II}} \simeq \hat{s}^{(n)}_{\mathrm{II}}$. □

Note that in case of multiple θ attempts, the above probability P satisfies

$$P = \prod_{i=1}^{n} \sum_{j=1}^{m_i} p_i\left(t'_{i-1}, u'_{i-1}\right)\left(1 - p_{i-1}\left(t'_{i-1}, u'_{i-1}\right)\right)^{(j-1)},$$

where m_i is the number of θ attempts at stage i. Finally, since Theorem 1 imposes no constraints on $move(\varrho)$, a DAG can simulate all proper executions that exist in the corresponding HIG.

Theorem 2 (DAG-HIG Simulation). *For any HIG $\mathcal{G}_\mathsf{H}$ there exists a DAG $\mathcal{G}_\mathsf{D} = \mathfrak{D}[\mathcal{G}_\mathsf{H}]$ such that $\mathcal{G}_\mathsf{D} \rightsquigarrow \mathcal{G}_\mathsf{H}$ (as defined in Definition 9).*

4 Properties of DAG and DAG-based Synthesis

We here discuss DAG features, including how it can be decomposed into subgames by restricting the simulation to finite executions, and the preservation of safety properties, before proposing a DAG-based synthesis framework.

Transitions. In DAGs, nondeterministic actions of different players underline different semantics. Specifically, PL_I nondeterminism captures what is known about the adversarial behavior, rather than exact actions, where PL_I actions are constrained by the earlier PL_II action. Conversely, PL_II nondeterminism abstracts the player's decisions. This distinction reflects how DAGs can be used for strategy synthesis under hidden information. To illustrate this, suppose that a strategy π_II is to be obtained based on a worst-case scenario. In that case, the game is explored for all possible adversarial behaviors. Yet, if a strategy π_I is known about PL_I, a counter strategy π_II can be found by constructing $\mathcal{G}_\text{D}^{\pi_\text{I}}$.

Probabilistic behaviors in DAGs are captured by $\text{PL}_\bigcirc$, which is characterized by the transition function $\hat{\delta}\colon \hat{S}_\bigcirc \times \hat{S}_\text{II} \to [0,1]$. The specific definition of $\hat{\delta}$ depends on the modeled system. For instance, if the transition function (i.e., the probability) is state-independent, i.e., $\hat{\delta}(\hat{s}_\bigcirc, \hat{s}_\text{II}) = c, c \in [0,1]$, the obtained model becomes trivial. Yet, with a state-dependent transition function, i.e., $\hat{\delta}(\hat{s}_\bigcirc, \hat{s}_\text{II}) = p(\hat{t}, \hat{u})$, the probability that PL_II successfully reveals the true value depends on both the belief and the true value, and the transition function can then be realized since $\hat{s}_\bigcirc$ holds both $\hat{t}$ and $\hat{u}$.

Decomposition. Consider an execution $\hat{\varrho}^* = \hat{s}_0 a_1 \hat{s}_1 a_2 \hat{s}_2 \dots$ that describes a scenario where PL_II performs infinitely many actions with no attempt to reveal the true value. To simulate $\hat{\varrho}^*$, the word w needs to infinitely grow. Since we are interested in finite executions, we impose *stopping criteria* on the DAG, such that the game is *trapped* whenever $|w| = h_\text{max}$ is true, where $h_\text{max} \in \mathbb{N}$ is an *upper horizon*. We formalize the stopping criteria as a deterministic finite automaton (DFA) that, when composed with the DAG, traps the game whenever the stopping criteria hold. Note that imposing an upper horizon by itself is not a sufficient criterion for a DAG to be considered a stopping game [8]. Conversely, consider a proper (and hence finite) execution $\hat{\varrho} = \hat{s}_0 a_1 \dots \hat{s}'$, where $\hat{s}_0, \hat{s}' \in \text{Prop}(\mathcal{G}_\text{D})$. From Definition 9, it follows that a DAG initial state is strictly proper, i.e., $\hat{s}_0 \in \text{Prop}(\mathcal{G}_\text{D})$. Hence, when $\hat{s}'$ is reached, the game can be seen as if it is *repeated* with a new initial state $\hat{s}'$. Consequently, a DAG game (complemented with stopping criteria) can be decomposed into a (possibly infinite) countable set of *subgames* that have the same structure yet different initial states.

Definition 10 (DAG Subgames). *The* subgames *of a* $\mathcal{G}_\text{D}$ *are defined by the set* $\left\{ \hat{\mathcal{G}}_i \;\middle|\; \hat{\mathcal{G}}_i = \left\langle \hat{S}^{(i)}, (\hat{S}_\text{I}^{(i)}, \hat{S}_\text{II}^{(i)}, \hat{S}_\bigcirc^{(i)}), A, \hat{s}_0^{(i)}, \hat{\delta}^{(i)} \right\rangle, i \in \mathbb{N}_0 \right\}$, *where* $\hat{S} = \bigcup_i \hat{S}^{(i)}$; $\hat{S}_\gamma = \bigcup_i \hat{S}_\gamma^{(i)}\ \forall \gamma \in \Gamma$; *and* $\hat{s}_0^{(i)} = \hat{s}_\text{II}^{(i)}$ *s.t.* $\hat{s}_\text{II}^{(i)} \in \text{Prop}(\mathcal{G}_\text{D}^{(i)})$, $\hat{s}_\text{II}^{(i)} \neq \hat{s}_\text{II}^{(j)}\ \forall i, j \in \mathbb{N}_0$.

Intuitively, each subgame either reaches a proper state (representing the initial state of another subgame) or terminates by an upper horizon. This decomposition allows for the independent (and parallel) analysis of individual subgames, drastically reducing both the time required for synthesis and the explored state space, and hence improving scalability. An example of this decompositional approach is provided in Sect. 5.

Preservation of Safety Properties. In DAGs, the action θ denotes a transition from PL_{II} to PL_{I} states and thus the execution of any delayed actions. While this action can simply describe a revealing attempt, it can also serve as a *what-if* analysis of how the true value may evolve at stage i of a subgame. We refer to an execution of the second type as a *hypothetical branch*, where $\text{Hyp}(\hat{\varrho}, h)$ denotes the set of hypothetical branches from $\hat{\varrho}$ at stage $h \in \{1, \ldots, n\}$. Let $L_{\text{safe}}(s)$ be a labeling function denoting if a state is safe. The formula $\Phi_{\text{safe}} \coloneqq [\mathsf{G}\, \mathit{safe}]$ is satisfied by an execution ϱ in HIG iff all $s(t, u, \Omega) \in \varrho$ are safe.

Now, consider $\hat{\varrho}$ of the DAG, with $\hat{\varrho} \sim \varrho$. We identify the following three cases:

(a) $L_{\text{safe}}(s)$ depends only on the belief u, then $\varrho \models \Phi_{\text{safe}}$ iff all $\hat{s}_{II} \in \hat{\varrho}$ are safe;
(b) $L_{\text{safe}}(s)$ depends only on the true value t, then $\varrho \models \Phi_{\text{safe}}$ iff all $\hat{s}_{\text{I}} \in \text{Hyp}(\hat{\varrho}, n)$ are safe; and
(c) $L_{\text{safe}}(s)$ depends on both the true value t and belief u, then $\varrho \models \Phi_{\text{safe}}$ iff $\mathit{last}(\hat{\varrho}_h)$ is safe for all $\hat{\varrho}_h \in \text{Hyp}(\hat{\varrho}, h), h \in \{1, ..., n\}$, where n is the number of PL_{II} actions.

Taking into account such relations, both safety (e.g., never encounter a hazard) and distance-based requirements (e.g., never exceed a subgame horizon) can be specified when using DAGs for synthesis, to ensure their satisfaction in the original model. This can be generalized to other reward-based synthesis objectives, which will be part of our future efforts that we discuss in Sect. 6.

Synthesis Framework. We here propose a framework for strategy synthesis using DAGs, which is summarized in Fig. 8. We start by formulating the automata $\mathcal{M}_{\text{I}}$, $\mathcal{M}_{\text{II}}$ and $\mathcal{M}_{\bigcirc}$, representing PL_{I}, PL_{II} and $\text{PL}_{\bigcirc}$ abstract behaviors, respectively. Next, a FIFO memory stack $(m_i)_{i=1}^{n} \in A_{\text{II}}^{n}$ is implemented using two automata $\mathcal{M}_{\text{mrd}}$ and $\mathcal{M}_{\text{mwr}}$ to perform reading and writing operations, respectively.[5] The DAG $\mathcal{G}_{\text{D}}$ is constructed by following Algorithm 1. The game starts with PL_{II} moves until she executes a revealing attempt θ, allowing PL_{I} to play her delayed actions. Once an end criterion is met, the game terminates, resembling conditions such as 'running out of fuel' or 'reaching map boundaries'.

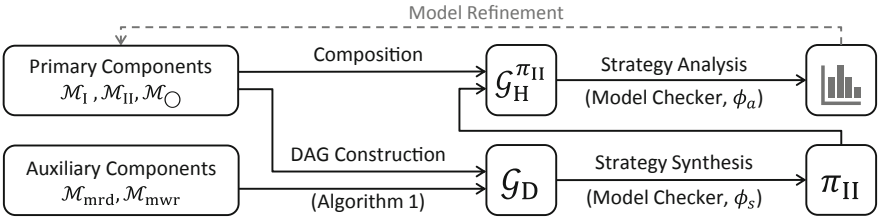


Fig. 8. Synthesis and analysis framework based on the use of DAGs.

[5] Specific implementation details are described in Sect. 5.

Algorithm 1. Procedure for DAG construction

Input: Components $\mathcal{M}_{\mathrm{I}}, \mathcal{M}_{\mathrm{II}}, \mathcal{M}_{\bigcirc}, \mathcal{M}_{\mathrm{mwr}}, \mathcal{M}_{\mathrm{mrd}}$; initial state $\hat{s}_0$
Result: DAG $\mathcal{G}_{\mathsf{D}}$

while $\neg(\textit{end criterion})$ **do**
  while $a \neq \theta$ **do** ▷ $\mathrm{PL}_{\mathrm{II}}$ plays until a revealing attempt
    $\mathcal{M}_{\mathrm{II}}.v_{\mathcal{B}} \leftarrow \textit{Eff}(a, v_{\mathcal{B}})$, $\mathcal{M}_{\mathrm{mwr}}.\textit{write}(a, \texttt{++}wr)$
  while $rd \leqslant wr$ **do** ▷ PL_{I} plays all delayed actions
    $\mathcal{M}_{\mathrm{mrd}}.\textit{read}(a, \texttt{++}rd)$, $\mathcal{M}_{\mathrm{I}}.v_{\mathcal{T}} \leftarrow \textit{Eff}(\beta(a), v_{\mathcal{T}})$
  if $\textit{draw}\ x \sim \textit{Brn}(p(v_{\mathcal{T}}, v_{\mathcal{B}}))$ **then** ▷ $\mathrm{PL}_{\bigcirc}$ plays successful attempt
    $\mathcal{M}_{\mathrm{II}}.v_{\mathcal{B}} \leftarrow \mathcal{M}_{\mathrm{I}}.v_{\mathcal{T}}$, $wr \leftarrow 0$, $rd \leftarrow 0$
  else $rd \leftarrow 0$ ▷ Unsuccessful attempt, forget PL_{I} actions

Algorithm 2 describes the procedure for strategy synthesis based on the DAG $\mathcal{G}_{\mathsf{D}}$, and an rPATL [6] synthesis query ϕ_{syn} that captures, for example, a safety requirement. Starting with the initial location, the procedure checks whether ϕ_{syn} is satisfied if action θ is performed at stage h, and updates the set of feasible strategies Π_i for subgame $\hat{\mathcal{G}}_i$ until $h_{\max}$ is reached or ϕ_{syn} is not satisfied.[6] Next, the set Π_i is used to update the list of reachable end locations ℓ with new initial locations of reachable subgames that should be explored. Finally, the composition of both $\mathcal{G}_{\mathsf{H}}$ and Π^*_{II} resolves $\mathrm{PL}_{\mathrm{II}}$ nondeterminism, where the resulting model $\mathcal{G}_{\mathsf{H}}^{\Pi^*_{\mathrm{II}}}$ is a Markov Decision Process (MDP) of complete information that can be easily used for further analysis.

5 Case Study

In this section, we consider a case study where a human operator supervises a UAV prone to stealthy attacks on its GPS sensor. The UAV mission is to visit a number of targets after being airborne from a known base (initial state), while avoiding hazard zones that are known a priori. Moreover, the presence of adversarial stealthy attacks via GPS spoofing is assumed. We use the DAG framework to synthesize strategies for both the UAV and an operator advisory system (AS) that schedules geolocation tasks for the operator.

Modeling. We model the system as a delayed-action game $\mathcal{G}_{\mathsf{D}}$, where PL_{I} and $\mathrm{PL}_{\mathrm{II}}$ represent the adversary and the UAV-AS coalition, respectively. Figure 9 shows the model primary and auxiliary components. In the UAV model $\mathcal{M}_{\mathrm{uav}}$, $x_{\mathcal{B}} = (\mathtt{x}_{\mathcal{B}}, \mathtt{y}_{\mathcal{B}})$ encodes the UAV belief, and $A_{\mathrm{uav}} = \{\mathsf{N}, \mathsf{S}, \mathsf{E}, \mathsf{W}, \mathsf{NE}, \mathsf{NW}, \mathsf{SE}, \mathsf{SW}\}$ is the set of available movements. The AS can trigger the action *activate* to initiate a geolocation task, attempting to confirm the current location. The adversary behavior is abstracted by $\mathcal{M}_{\mathrm{adv}}$ where $x_{\mathcal{T}} = (\mathtt{x}_{\mathcal{T}}, \mathtt{y}_{\mathcal{T}})$ encodes the UAV true location. The adversarial actions are limited to one directional

[6] Failing to find a strategy at stage i implies the same for all horizons of size $j > i$.

Algorithm 2. Procedure for strategy synthesis

Input: Initial location (x_0, y_0), synthesis query ϕ_{syn}
Output: PL_{II} strategies Π^*_{II}

$\ell \leftarrow [(x_0, y_0)]$, $i \leftarrow 0$
while $i < |\ell|$ **do** ▷ Explore all reachable subgames
  $\hat{s}_0 \leftarrow (\ell[i], \ell[i], \epsilon, 0, \text{II})$, $h \leftarrow 1$, $stop \leftarrow \bot$ ▷ Construct initial state
  while $h \leqslant h_{\max} \wedge \neg stop$ **do** ▷ Explore subgame till upper horizon
    $(\pi_{\text{II}}, \varphi) \leftarrow \mathsf{Synth}\left(\hat{\mathcal{G}}^{\pi_h}_{\hat{s}_0}, \phi_{\text{syn}}\right)$ ▷ Synthesize strategy for horizon h
    if $\pi_{\text{II}} \neq \emptyset$ **then**
      $\Pi_i \leftarrow \Pi_i \cup (\pi_{\text{II}}, \pi_h, \varphi)$, h++ ▷ Save synthesized strategy
    else $stop \leftarrow \top$
  $\mathsf{Prune}(\Pi_t)$, $\Pi^*_{\text{II}} \leftarrow \Pi^*_{\text{II}} \cup \Pi_t$ ▷ Prune subgame strategies
  $\ell \leftarrow \ell \cdot (\mathsf{Reachable}(\Pi_t) \setminus \ell)$, i++ ▷ update reachability

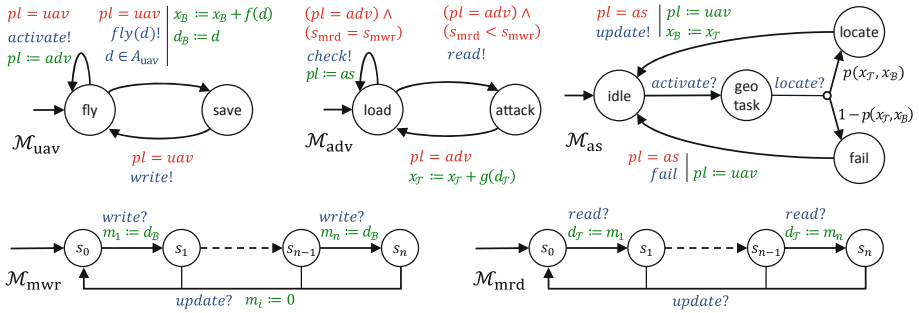


Fig. 9. Primary DAG components: UAV ($\mathcal{M}_{\text{uav}}$), adversary ($\mathcal{M}_{\text{adv}}$), and AS ($\mathcal{M}_{\text{as}}$). Auxiliary DAG components: memory write ($\mathcal{M}_{\text{mwr}}$) and memory read ($\mathcal{M}_{\text{mrd}}$) models, capturing the DAG representation. At stage i, the next memory location to write/read is m_i.

increment at most.[7] If, for example, the UAV is heading N, then the adversary set of actions is $\beta(\mathsf{N}) = \{\mathsf{N}, \mathsf{NE}, \mathsf{NW}\}$. The auxiliary components $\mathcal{M}_{\text{mwr}}$ and $\mathcal{M}_{\text{mrd}}$ manage a FIFO memory stack $(m_i)_{i=0}^{n-1} \in A^n_{\text{uav}}$. The last UAV movement is saved in m_i by synchronizing $\mathcal{M}_{\text{mwr}}$ with $\mathcal{M}_{\text{uav}}$ via *write*, while $\mathcal{M}_{\text{mrd}}$ synchronizes with $\mathcal{M}_{\text{adv}}$ via *read* to read the next UAV action from m_j. The subgame terminates whenever action *write* is attempted and $\mathcal{M}_{\text{mwr}}$ is at state n (i.e., out of memory).

The goal is to find strategies for the UAV-AS coalition based on the following:

– *Target reachability.* To overcome cases where targets are unreachable due to hazard zones, the label *reach* is assigned to the set of states with acceptable checkpoint locations (including the target) to render the objective incremen-

[7] To detect aggressive attacks, techniques from literature (e.g., [16,25,26]) can be used.

tally feasible. The objective for all encountered subgames is then formalized as $\Pr_{\max}[\mathsf{F}\ \mathit{reach}] \geqslant p_{\min}$ for some bound $p_{\min}$.
- *Hazard Avoidance.* Similar to target reachability, the label *hazard* is assigned to states corresponding to hazard zones. The objective $\Pr_{\max}[\mathsf{G}\ \neg \mathit{hazard}] \geqslant p_{\min}$ is then specified for all encountered subgames.

By refining the aforementioned objectives, synthesis queries are used for both the subgames and the supergame. Specifically, the query

$$\phi_{\text{syn}}(k) \coloneqq \langle\langle \text{uav} \rangle\rangle \Pr_{\max=?}\left[\neg \mathit{hazard}\ \mathsf{U}^{\leqslant k}\ (\mathit{locate} \wedge \mathit{reach})\right] \tag{1}$$

is specified for each encountered subgame $\hat{\mathcal{G}}_i$, where *locate* indicates a successful geolocation task. By following Algorithm 2 for a q number of reachable subgames, the supergame is reduced to an MDP $\mathcal{G}_{\mathsf{D}}^{\{\pi_i\}_{i=1}^{q}}$ (whose states are the reachable subgames), which is checked against the query

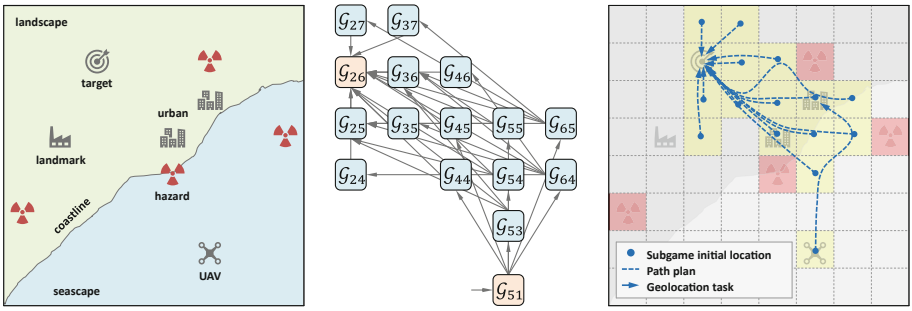
$$\phi_{\text{ana}}(n) \coloneqq \langle\langle \text{adv} \rangle\rangle \Pr_{\min,\max=?}\left[\mathsf{F}^{\leqslant n}\ \mathit{target}\right] \tag{2}$$

to find the bounds on the probability that the target is reached under a maximum number of geolocation tasks n.

Experimental Results. Figure 10(a) shows the map setting used for implementation. The UAV's ability to actively detect an attack depends on both its belief and the ground truth. Specifically, the probability of success in a geolocation task mainly relies on the disparity between the belief and true locations, captured by $f_{\text{dis}}\colon \mathit{Ev}\,(x_{\mathcal{B}}) \times \mathit{Ev}\,(x_{\mathcal{T}}) \rightarrow [0,1]$, obtained by assigning probabilities for each pair of locations according to their features (e.g., landmarks) and smoothed using a Gaussian 2D filter. A thorough experimental analysis where probabilities are extracted from experiments with human operators is described in [11]. The set of hazard zones include the map boundaries to prevent the UAV from reaching boundary values. Also, the adversary is prohibited from launching attacks for at least the first step, a practical assumption to prevent the UAV model from infinitely bouncing around the target location.

We implemented the model in PRISM-games [7,19] and performed the experiments on an Intel Core i7 4.0 GHz CPU, with 10 GB RAM dedicated to the tool. Figure 10(b) shows the supergame obtained by following the procedure in Algorithm 2. A vertex $\hat{\mathcal{G}}_{\mathtt{xy}}$ represents a subgame (composed with its strategy) that starts at location $(\mathtt{x}, \mathtt{y})$, while the outgoing edges points to subgames reachable from the current one. Note that each edge represents a probabilistic transition. Subgames with more than one outgoing transition imply nondeterminism that is resolved by the adversary actions. Hence, the directed graph depicts an MDP.

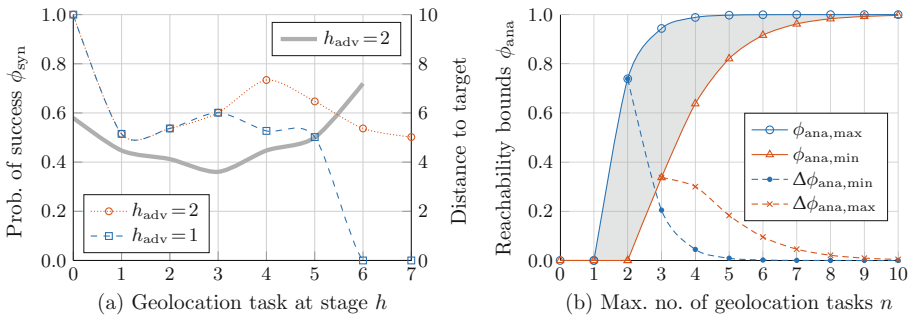
The synthesized strategy for $(h_{\text{adv}} = 2, h = 4)$ is demonstrated in Fig. 10(c). For the initial subgame, Fig. 11(a) shows the maximum probability of a successful geolocation task if performed at stage h, and the remaining distance to target. Assuming the adversary can launch attacks after stage $h_{\text{adv}} = 2$, the detection probability is maximized by performing the geolocation task at step 4,



(a) Environment setup. (b) Supergame $\mathcal{G}_{\mathrm{D}}$. (c) Protocols.

Fig. 10. (a) The environment setup used for the case study; (b) the induced supergame MDP, where the subgames form its states; and (c) the synthesized protocols.

and hazard areas can still be avoided up till $h = 6$. For $h_{\mathrm{adv}} = 1$, however, $h = 3$ has the highest probability of success, which diminishes at $h = 6$ as no possible flight plan exists without encountering a hazard zone. The effect of the maximum number of geolocation tasks (n) on target reachability is studied by analyzing the supergame against ϕ_{ana} as shown in Fig. 11(b). The minimum number of geolocation tasks to guarantee a non-zero probability of reaching the target (regardless of the adversary strategy) is 3 with probability bounds of $(33.7\%, 94.4\%)$.



(a) Geolocation task at stage h (b) Max. no. of geolocation tasks n

Fig. 11. Analysis results for (a) subgame $\hat{\mathcal{G}}_{51}$ and (b) supergame $\mathcal{G}_{\mathrm{D}}$.

The experimental data obtained for this case study are listed in Table 1. For the same grid size, more complex maps require more time for synthesis while the state space size remains unaffected. The state space grows exponentially with the explored horizon size, i.e., $\mathcal{O}\left((|A_{\mathrm{uav}}||A_{\mathrm{adv}}|)^h\right)$, and is typically slowed by, e.g., the presence of hazard areas, since the branches of the game transitions are trimmed upon encountering such areas. Interestingly, for $h = 6$ and $h = 7$,

while the model construction time (size) for $h_{\text{adv}} = 1$ is almost twice (quadruple) as those for $h_{\text{adv}} = 2$, the time for checking ϕ_{syn} declines in comparison. This reflects the fact that, in case of $h_{\text{adv}} = 1$ compared to $h_{\text{adv}} = 2$, the UAV has higher chances to reach a hazard zone for the same k, leading to a shorter time for model checking.

Table 1. Results for strategy synthesis using queries ϕ_{syn} and ϕ_{ana}.

Subgame $\hat{\mathcal{G}}_{51}$			Model size			Time (sec)		
Map	t_{adv}	k	States	Transitions	Choices	Model	ϕ_{syn}	ϕ_{ana}
8×8	1	4	11,608	17,397	15,950	2.810	0.072	–
		5	57,129	87,865	83,267	14.729	0.602	–
		6	236,714	366,749	359,234	62.582	1.293	–
		7	876,550	1,365,478	1,355,932	231.741	6.021	–
	2	4	6,678	9,230	8,394	2.381	0.042	–
		5	33,904	48,545	45,354	10.251	0.367	–
		6	141,622	204,551	198,640	37.192	1.839	–
		7	524,942	763,144	754,984	145.407	8.850	–
Supergame $\mathcal{G}_{\text{D}}$			6,212	8,306	6,660	2.216	–	2.490

6 Discussion and Conclusion

In this paper, we introduced DAGs and showed how they can simulate HIGs by delaying players' actions. We also derived a DAG-based framework for strategy synthesis and analysis using off-the-shelf SMG model checkers. Under some practical assumptions, we showed that DAGs can be decomposed into independent subgames, utilizing parallel computation to reduce the time needed for model analysis, as well as the size of the state space. We further demonstrated the applicability of the proposed framework on a case study focused on synthesis and analysis of active attack detection strategies for UAVs prone to cyber attacks.

DAGs come at the cost of increasing the total state space size as $\mathcal{M}_{\text{mrd}}$ and $\mathcal{M}_{\text{mwr}}$ are introduced. This does not present a significant limitation due to the compositional approach towards strategy synthesis using subgames. However, the synthesis is still limited to model sizes that off-the-shelf tools can handle.

The concept of delaying actions implicitly assumes that the adversary knows the UAV actions a priori. This does not present a concern in the presented case study as an abstract (i.e., nondeterministic) adversary model is analogous to synthesizing against the worst-case attacking scenario. Nevertheless, strategies synthesized using DAGs (and SMGs in general) are inherently conservative. Depending on the considered system, this can easily lead to no feasible solution.

The proposed synthesis framework ensures preservation of safety properties. Yet, general reward-based strategy synthesis is to be approached with care. For example, rewards dependent on the belief can appear in any state, and exploring hypothetical branches is not required. However, rewards dependent on a state's true value should only appear in proper states, and all hypothetical branches are to be explored. A detailed investigation of how various properties are preserved by DAGs, along with multi-objective synthesis, is a direction for future work.

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Automated Hypersafety Verification

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Abstract. We propose an automated verification technique for hypersafety properties, which express sets of valid interrelations between multiple finite runs of a program. The key observation is that constructing a proof for a small representative set of the runs of the product program (i.e. the product of the several copies of the program by itself), called a *reduction*, is sufficient to formally prove the hypersafety property about the program. We propose an algorithm based on a counterexample-guided refinement loop that simultaneously searches for a reduction and a proof of the correctness for the reduction. We demonstrate that our tool Weaver is very effective in verifying a diverse array of hypersafety properties for a diverse class of input programs.

1 Introduction

A hypersafety property describes the set of valid interrelations between multiple finite runs of a program. A k-safety property [7] is a program safety property whose violation is witnessed by at least k finite runs of a program. Determinism is an example of such a property: non-determinism can only be witnessed by two runs of the program on the same input which produce two different outputs. This makes determinism an instance of a 2-safety property.

The vast majority of existing program verification methodologies are geared towards verifying standard (1-)safety properties. This paper proposes an approach to automatically reduce verification of k-safety to verification of 1-safety, and hence a way to leverage existing safety verification techniques for hypersafety verification. The most straightforward way to do this is via *self-composition* [5], where verification is performed on k memory-disjoint copies of the program, sequentially composed one after another. Unfortunately, the proofs in these cases are often very verbose, since the full functionality of each copy has to be captured by the proof. Moreover, when it comes to automated verification, the invariants required to verify such programs are often well beyond the capabilities of modern solvers [26] even for very simple programs and properties.

The more practical approach, which is typically used in manual or automated proofs of such properties, is to compose k memory-disjoint copies of the program *in parallel* (instead of in sequence), and then verify some *reduced* program obtained by removing redundant traces from the program formed in the previous step. This parallel product program can have many such reductions.

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For example, the program formed from sequential self-composition is one such reduction of the parallel product program. Therefore, care must be taken to choose a "good" reduction that *admits a simple proof*. Many existing approaches limit themselves to a narrow class of reductions, such as the one where each copy of the program executes in lockstep [3,10,24], or define a general class of reductions, but do not provide algorithms with guarantees of covering the entire class [4,24].

We propose a solution that combines the search for a safety proof with the search for an appropriate reduction, in a counterexample-based refinement loop. Instead of settling on a single reduction in advance, we try to verify the entire (possibly infinite) set of reductions simultaneously and terminate as soon as some reduction is successfully verified. If the proof is not currently strong enough to cover at least one of the represented program reductions, then an appropriate set of counterexamples are generated that guarantee progress towards a proof.

Our solution is language-theoretic. We propose a way to represent sets of reductions using infinite tree automata. The standard safety proofs are also represented using the same automata, which have the desired closure properties. This allows us to check if a candidate proof is in fact a proof for one of the represented program reductions, with reasonable efficiency.

Our approach is not uniquely applicable to hypersafety properties of sequential programs. Our proposed set of reductions naturally work well for concurrent programs, and can be viewed in the spirit of reduction-based methods such as those proposed in [11,21]. This makes our approach particularly appealing when it comes to verification of hypersafety properties of concurrent programs, for example, proving that a concurrent program is deterministic. The parallel composition for hypersafety verification mentioned above and the parallel composition of threads inside the multi-threaded program are treated in a uniform way by our proof construction and checking algorithms. In summary:

- We present a counterexample-guided refinement loop that simultaneously searches for a proof and a program reduction in Sect. 7. This refinement loop relies on an efficient algorithm for proof checking based on the antichain method of [8], and strong theoretical progress guarantees.
- We propose an automata-based approach to representing a class of program reductions for k-safety verification. In Sect. 5 we describe the precise class of automata we use and show how their use leads to an effective proof checking algorithm incorporated in our refinement loop.
- We demonstrate the efficacy of our approach in proving hypersafety properties of sequential and concurrent benchmarks in Sect. 8.

2 Illustrative Example

We use a simple program Mult, that computes the product of two non-negative integers, to illustrate the challenges of verifying hypersafety properties and the type of proof that our approach targets. Consider the multiplication program in Fig. 1(i), and assume we want to prove that it is distributive over addition.

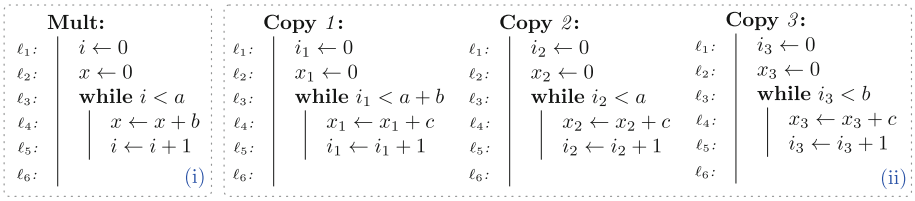

Fig. 1. Program MULT (i) and the parallel composition of three copies of it (ii).

In Fig. 1(ii), the parallel composition of MULT with two copies of itself is illustrated. The product program is formed for the purpose of proving distributivity, which can be encoded through the postcondition $x_1 = x_2 + x_3$. Since a, b, and c are not modified in the program, the same variables are used across all copies. One way to prove MULT is distributive is to come up with an inductive invariant ϕ_{ijk} for each location in the product program, represented by a triple of program locations (ℓ_i, ℓ_j, ℓ_k), such that $\mathit{true} \implies \phi_{111}$ and $\phi_{666} \implies x_1 = x_2 + x_3$. The main difficulty lies in finding assignments for locations such as ϕ_{611} that are points in the execution of the program where one thread has finished executing and the next one is starting. For example, at (ℓ_6, ℓ_1, ℓ_1) we need the assignment $\phi_{611} \leftarrow x_1 = (a + b) * c$ which is non-linear. However, the program given in Fig. 1(ii) can be verified with simpler (linear) reasoning.

The program on the right is a semantically equivalent *reduction* of the full composition of Fig. 1(ii). Consider the program P = (Copy 1 || (Copy 2; Copy 3)). The program on the right is equivalent to a lockstep execution of the two parallel components of P. The validity of this reduction is derived from the fact that the statements in each thread are *independent* of the statements in the other. That is, reordering the statements of different threads in an execution leads to an equivalent execution. It is easy to see that $x_1 = x_2 + x_3$ is an invariant of both while loops in the reduced program, and therefore, linear reasoning is sufficient to prove the postcondition for this program. Conceptually, this reduction (and its soundness proof) together with the proof of correctness for the reduced program constitute a proof that the original program MULT is distributive. Our proposed approach can come up with reductions like this and their corresponding proofs fully automatically. Note that a lockstep reduction of the program in Fig. 1(ii) would not yield a solution for this problem and therefore the discovery of the right reduction is an integral part of the solution.

$i_1 \leftarrow 0,\ i_2 \leftarrow 0,\ i_3 \leftarrow 0$
$x_1 \leftarrow 0,\ x_2 \leftarrow 0,\ x_3 \leftarrow 0$
while $i_2 < a$
  $x_1 \leftarrow x_1 + c$
  $x_2 \leftarrow x_2 + c$
  $i_1 \leftarrow i_1 + 1$
  $i_2 \leftarrow i_2 + 1$
while $i_3 < b$
  $x_1 \leftarrow x_1 + c$
  $x_3 \leftarrow x_3 + c$
  $i_1 \leftarrow i_1 + 1$
  $i_3 \leftarrow i_3 + 1$

3 Programs and Proofs

A non-deterministic finite automaton (NFA) is a tuple $A = (Q, \Sigma, \delta, q_0, F)$ where Q is a finite set of states, Σ is a finite alphabet, $\delta \subseteq Q \times \Sigma \times Q$ is the transition relation, $q_0 \in Q$ is the initial state, and $F \subseteq Q$ is the set of final states. A deterministic finite automaton (DFA) is an NFA whose transition relation is a function $\delta : Q \times \Sigma \to Q$. The language of an NFA or DFA A is denoted $\mathcal{L}(A)$, which is defined in the standard way [18].

3.1 Program Traces

$\mathcal{S}t$ denotes the (possibly infinite) set of *program states*. For example, a program with two integer variables has $\mathcal{S}t = \mathbb{Z} \times \mathbb{Z}$. $\mathcal{A} \subseteq \mathcal{S}t$ is a (possibly infinite) set of *assertions* on program states. Σ denotes a finite alphabet of program *statements*. We refer to a finite string of statements as a (program) *trace*. For each statement $a \in \Sigma$ we associate a *semantics* $[\![a]\!] \subseteq \mathcal{S}t \times \mathcal{S}t$ and extend $[\![-]\!]$ to traces via (relation) composition. A trace $x \in \Sigma^*$ is said to be *infeasible* if $[\![x]\!](\mathcal{S}t) = \emptyset$, where $[\![x]\!](\mathcal{S}t)$ denotes the image of $[\![x]\!]$ under $\mathcal{S}t$. To abstract away from a particular program syntax, we define a *program* as a regular language of traces. The semantics of a program P is simply the union of the semantics of its traces $[\![P]\!] = \bigcup_{x \in P} [\![x]\!]$. Concretely, one may obtain programs as languages by interpreting their edge-labelled control-flow graphs as DFAs: each vertex in the control flow graph is a state, and each edge in the control flow graph is a transition. The control flow graph entry location is the initial state of the DFA and all its exit locations are final states.

3.2 Safety

There are many equivalent notions of program safety; we use non-reachability. A program P is *safe* if all traces of P are infeasible, i.e. $[\![P]\!](\mathcal{S}t) = \emptyset$. Standard partial correctness specifications are then represented via a simple encoding. Given a precondition ϕ and a postcondition ψ, the validity of the Hoare-triple $\{\phi\}P\{\psi\}$ is equivalent to the safety of $[\phi] \cdot P \cdot [\neg\psi]$, where [] is a standard assume statement (or the singleton set containing it), and $\cdot$ is language concatenation.

Example 3.1. We use determinism as an example of how k-safety can be encoded in the framework defined thus far. If P is a program then determinism of P is equivalent to safety of $[\phi] \cdot (P_1 \sqcup\!\sqcup P_2) \cdot [\neg\phi]$ where P_1 and P_2 are copies of P operating on disjoint variables, $\sqcup\!\sqcup$ is a shuffle product of two languages, and $[\phi]$ is an assume statement asserting that the variables in each copy of P are equal.

A *proof* is a finite set of assertions $\Pi \subseteq \mathcal{A}$ that includes *true* and *false*. Each Π gives rise to an NFA $\Pi_{NFA} = (\Pi, \mathcal{S}t, \delta_\Pi, \mathit{true}, \{\mathit{false}\})$ where $\delta_\Pi(\phi_{pre}, a) = \{\phi_{post} \mid [\![a]\!](\phi_{pre}) \subseteq \phi_{post}\}$. We abbreviate $\mathcal{L}(\Pi_{NFA})$ as $\mathcal{L}(\Pi)$. Intuitively, $\mathcal{L}(\Pi)$

consists of all traces that can be proven infeasible using only assertions in Π. Thus the following proof rule is sound [12,13,17]:

$$\frac{\exists \Pi \subseteq \mathcal{A}.\, P \subseteq \mathcal{L}(\Pi)}{P \text{ is safe}} \qquad (\textsc{Safe})$$

When $P \subseteq \mathcal{L}(\Pi)$, we say that Π is a proof for P. A proof does not uniquely belong to any particular program; a single Π may prove many programs correct.

4 Reductions

The set of assertions used for a proof is usually determined by a particular language of assertions, and a safe program may not have a (safety) proof in that particular language. Yet, a subset of the program traces may have a proof in that assertion language. If it can be proven that the subset of program runs that have a safety proof are a faithful representation of all program behaviours (with respect to a given property), then the program is correct. This motivates the notion of *program reductions*.

Definition 4.1 (semantic reduction). *If for programs P and P', P' is safe implies that P is safe, then P' is a* semantic reduction *of P (written $P' \preceq P$).*

The definition immediately gives rise to the following proof rule for proving program safety:

$$\frac{\exists P' \preceq P, \Pi \subseteq \mathcal{A}.\, P' \subseteq \mathcal{L}(\Pi)}{P \text{ is safe}} \qquad (\textsc{SafeRed}1)$$

This generic proof rule is not automatable since, given a proof Π, verifying the existence of the appropriate reduction is *undecidable*. Observe that a program is safe if and only if $\emptyset$ is a valid reduction of the program. This means that discovering a semantic reduction and proving safety are mutually reducible to each other. To have decidable premises for the proof rule, we need to formulate an easier (than proving safety) problem in discovering a reduction. One way to achieve this is by restricting the set of reductions under consideration from all reductions (given in Definition 4.1) to a proper subset which more amenable to algorithmic checking. Fixing a set $\mathcal{R}$ of (semantic) reductions, we will have the rule:

$$\frac{\exists P' \in \mathcal{R}.\, P' \subseteq \mathcal{L}(\Pi) \qquad \forall P' \in \mathcal{R}.\, P' \preceq P}{P \text{ is safe}} \qquad (\textsc{SafeRed}2)$$

Proposition 4.2. *The proof rule* SafeRed2 *is sound.*

The core contribution of this paper is that it provides an algorithmic solution inspired by the above proof rule. To achieve this, two subproblems are solved: (1) Given a set $\mathcal{R}$ of reductions of a program P and a candidate proof Π, can we check if there exists a reduction $P' \in \mathcal{R}$ which is covered by the proof Π? In Sect. 5, we propose a new semantic interpretation of an existing notion of infinite tree automata that gives rise to an algorithmic check for this step. (2) Given a program P, is there a general sound set of reductions $\mathcal{R}$ that be effectively represented to accommodate step (1)? In Sect. 6, we propose a construction of an effective set of reductions, representable by our infinite tree automata, using inspirations from existing partial order reduction techniques [15].

5 Proof Checking

Given a set of reductions $\mathcal{R}$ of a program P, and a candidate proof Π, we want to check if there exists a reduction $P' \in \mathcal{R}$ which is covered by Π. We call this *proof checking*. We use tree automata to represent certain classes of languages (i.e sets of sets of strings), and then use operations on these automata for the purpose of proof checking.

The set Σ^* can be represented as an infinite tree. Each $x \in \Sigma^*$ defines a path to a unique node in the tree: the root node is located at the empty string ϵ, and for all $a \in \Sigma$, the node located at xa is a child of the node located at x. Each node is then identified by the string labeling the path leading to it. A language $L \subseteq \Sigma^*$ (equivalently, $L : \Sigma^* \to \mathbb{B}$) can consequently be represented as an infinite tree where the node at each x is labelled with a boolean value $B \equiv (x \in L)$. An example is given in Fig. 2.

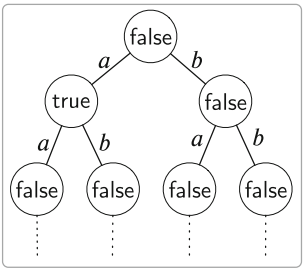

Fig. 2. Language $\{a\}$ as an infinite tree.

It follows that a set of languages is a set of infinite trees, which can be represented using automata over infinite trees. Looping Tree Automata (LTAs) are a subclass of Büchi Tree Automata where all states are accept states [2]. The class of Looping Tree Automata is closed under intersection and union, and checking emptiness of LTAs is decidable. Unlike Büchi Tree Automata, emptiness can be decided in linear time [2].

Definition 5.1. *A Looping Tree Automaton (LTA) over $|\Sigma|$-ary, $\mathbb{B}$-labelled trees is a tuple $M = (Q, \Delta, q_0)$ where Q is a finite set of states, $\Delta \subseteq Q \times \mathbb{B} \times (\Sigma \to Q)$ is the transition relation, and q_0 is the initial state.*

Intuitively, an LTA $M = (Q, \Delta, q_0)$ performs a parallel and depth-first traversal of an infinite tree L while maintaining some local state. Execution begins at the root ϵ from state q_0 and non-deterministically picks a transition $(q_0, B, \sigma) \in \Delta$ such that B matches the label at the root of the tree (i.e. $B = (\epsilon \in L)$). If no such transition exists, the tree is rejected. Otherwise, M recursively works on

each child a from state $q' = \sigma(a)$ in parallel. This process continues infinitely, and L is accepted if and only if L is never rejected.

Formally, M's execution over a tree L is characterized by a *run* $\delta^* : \Sigma^* \rightarrow Q$ where $\delta^*(\epsilon) = q_0$ and $(\delta^*(x), x \in L, \lambda a.\, \delta^*(xa)) \in \Delta$ for all $x \in \Sigma^*$. The set of languages accepted by M is then defined as $\mathcal{L}(M) = \{L \mid \exists \delta^*.\, \delta^*$ is a run of M on $L\}$.

Theorem 5.2. *Given an LTA M and a regular language L, it is decidable whether $\exists P \in \mathcal{L}(M).\, P \subseteq L$.*

The proof, which appears in [14], reduces the problem to deciding whether $\mathcal{L}(M) \cap \mathcal{P}(L) \neq \emptyset$. LTAs are closed under intersection and have decidable emptiness checks, and the lemma below is the last piece of the puzzle.

Lemma 5.3. *If L is a regular language, then $\mathcal{P}(L)$ is recognized by an LTA.*

Counterexamples. Theorem 5.2 effectively states that proof checking is decidable. For automated verification, beyond checking the validity of a proof, we require counterexamples to fuel the development of the proof when the proof does not check. Note that in the simple case of the proof rule SAFE, when $P \not\subseteq \mathcal{L}(\Pi)$ there exists a counterexample trace $x \in P$ such that $x \notin \mathcal{L}(\Pi)$.

With our proof rule SafeRed2, things get a bit more complicated. First, note that unlike the classic case (SAFE), where a failed proof check coincides with the non-emptiness of an intersection check (i.e. $P \cap \overline{\mathcal{L}(\Pi)} \neq \emptyset$), in our case, a failed proof check coincides with the emptiness of an intersection check (i.e. $\mathcal{R} \cap \mathcal{P}(\mathcal{L}(\Pi)) = \emptyset$). The sets $\mathcal{R}$ and $\mathcal{P}(\mathcal{L}(\Pi))$ are both sets of languages. What does the witness to the emptiness of the intersection look like? Each language member of $\mathcal{R}$ contains at least one string that does not belong to any of the subsets of our proof language. One can collect all such witness strings to guarantee progress across the board in the next round. However, since LTAs can represent an infinite set of languages, one must take care not end up with an infinite set of counterexamples following this strategy. Fortunately, this will not be the case.

Theorem 5.4. *Let M be an LTA and let L be a regular language such that $P \not\subseteq L$ for all $P \in \mathcal{L}(M)$. There exists a finite set of counterexamples C such that, for all $P \in \mathcal{L}(M)$, there exists some $x \in C$ such that $x \in P$ and $x \notin L$.*

The proof appears in [14]. This theorem justifies our choice of using LTAs instead of more expressive formalisms such as Büchi Tree Automata. For example, the Büchi Tree Automaton that accepts the language $\{\{x\} \mid x \in \Sigma^*\}$ would give rise to an infinite number of counterexamples with respect to the empty proof (i.e. $\Pi = \emptyset$). The finiteness of the counterexample set presents an alternate proof that LTAs are strictly less expressive than Büchi Tree Automata [27].

6 Sleep Set Reductions

We have established so far that (1) a set of assertions gives rise to a regular language proof, and (2) given a regular language proof and a set of program reductions recognizable by an LTA, we can check the program (reductions) against the proof. The last piece of the puzzle is to show that a useful class of program reductions can be expressed using LTAs.

Recall our example from Sect. 2. The reduction we obtain is sound because, for every trace in the full parallel-composition program, an equivalent trace exists in the reduced program. By equivalent, we mean that one trace can be obtained from the other by swapping independent statements. Such an equivalence is the essence of the theory of Mazurkiewicz traces [9].

We fix a reflexive symmetric *dependence relation* $D \subseteq \Sigma \times \Sigma$. For all $a, b \in \Sigma$, we say that a and b are *dependent* if $(a, b) \in D$, and say they are *independent* otherwise. We define $\sim_D$ as the smallest congruence satisfying $xaby \sim_D xbay$ for all $x, y \in \Sigma^*$ and independent $a, b \in \Sigma$. The closure of a language $L \subseteq \Sigma^*$ with respect to $\sim_D$ is denoted $[L]_D$. A language L is $\sim_D$*-closed* if $L = [L]_D$. It is worthwhile to note that all input programs considered in this paper correspond to regular languages that are $\sim_D$-closed.

An equivalence class of $\sim_D$ is typically called a (Mazurkiewicz) trace. We avoid using this terminology as it conflicts with our definition of traces as strings of statements in Sect. 3.1. We assume D is *sound*, i.e. $[\![ab]\!] = [\![ba]\!]$ for all independent $a, b \in \Sigma$.

Definition 6.1 (D-reduction). *A program P' is a* D-reduction *of a program P, that is $P' \preceq_D P$, if $[P']_D = P$.*

Note that the equivalence relation on programs induced by $\sim_D$ is a refinement of the semantic equivalence relation used in Definition 4.1.

Lemma 6.2. *If $P' \preceq_D P$ then $P' \preceq P$.*

Ideally, we would like to define an LTA that accepts all D-reductions of a program P, but unfortunately this is not possible in general.

Proposition 6.3 (corollary of Theorem 67 of [9]). *For arbitrary regular languages $L_1, L_2 \in \Sigma^*$ and relation D, the proposition $\exists L \preceq_D L_1 . L \subseteq L_2$ is undecidable.*

The proposition is decidable only when $\overline{D}$ is transitive, which does not hold for a semantically correct notion of independence for a parallel program encoding a k-safety property, since statements from the same thread are dependent and statements from different program copies are independent. Therefore, we have:

Proposition 6.4. *Assume P is a $\sim_D$-closed program and Π is a proof. The proposition $\exists P' \preceq_D P . P' \subseteq \mathcal{L}(\Pi)$ is undecidable.*

In order to have a decidable premise for proof rule SafeRed2 then, we present an approximation of the set of D-reductions, inspired by sleep sets [15]. The idea is to construct an LTA that recognizes *a class of D-reductions* of an input program P, whose language is assumed to be $\sim_D$-closed. This automaton intuitively makes non-deterministic choices about what program traces to *prune* in favour of other $\sim_D$-equivalent program traces for a given reduction. Different non-deterministic choices lead to different D-reductions.

Consider two statements $a, b \in \Sigma$ where $(a, b) \notin D$. Let $x, y \in \Sigma^*$ and consider two program runs $xaby$ and $xbay$. We know $[\![xbay]\!] = [\![xaby]\!]$. If the automaton makes a non-deterministic choice that the successors of xa have been explored, then the successors of xba need not be explored (can be pruned away) as illustrated in Fig. 3. Now assume $(a, c) \in D$, for some $c \in \Sigma$. When the node xbc is being explored, we can no longer safely ignore a-transitions, since the equality $[\![xbcay]\!] = [\![xabcy]\!]$ is not guaranteed. Therefore, the a successor of xbc has to be explored. The nondeterministic choice of what child node to explore is modelled by a choice of order in which we explore each node's children. Different orders yield different reductions. Reductions are therefore characterized as an assignment $R : \Sigma^* \to \mathcal{L}in(\Sigma)$ from nodes to linear orderings on Σ, where $(a, b) \in R(x)$ means we explore child xa after child xb.

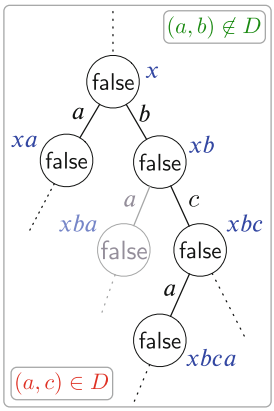

Fig. 3. Exploring from x with sleep sets.

Given $R : \Sigma^* \to \mathcal{L}in(\Sigma)$, the *sleep set* $\text{sleep}_R(x) \subseteq \Sigma$ at node $x \in \Sigma^*$ defines the set of transitions that can be ignored at x:

$$\text{sleep}_R(\epsilon) = \emptyset \tag{1}$$

$$\text{sleep}_R(xa) = (\text{sleep}_R(x) \cup R(x)(a)) \setminus D(a) \tag{2}$$

Intuitively, (1) no transition can be ignored at the root node, since nothing has been explored yet, and (2) at node x, the sleep set of xa is obtained by adding the transitions we explored before a ($R(x)(a)$) and then removing the ones that conflict with a (i.e. are related to a by D). Next, we define the nodes that are ignored. The set of ignored nodes is the smallest set $\text{ignore}_R : \Sigma^* \to \mathbb{B}$ such that

$$x \in \text{ignore}_R \implies xa \in \text{ignore}_R \tag{1}$$

$$a \in \text{sleep}_R(x) \implies xa \in \text{ignore}_R \tag{2}$$

Intuitively, a node xa is ignored if (1) any of its ancestors is ignored ($\text{ignore}_R(x)$), or (2) a is one of the ignored transitions at node x ($a \in \text{sleep}_R(x)$).

Finally, we obtain an actual reduction of a program P from a characterization of a reduction R by removing the ignored nodes from P, i.e. $P \setminus \text{ignore}_R$.

Lemma 6.5. *For all $R : \Sigma^* \to \mathcal{L}in(\Sigma)$, if P is a $\sim_D$-closed program then $P \setminus \text{ignore}_R$ is a D-reduction of P.*

The set of all such reductions is $\text{reduce}_D(P) = \{P \backslash \text{ignore}_R \mid R : \Sigma^* \to \mathcal{L}in(\Sigma)\}$.

Theorem 6.6. *For any regular language P, $\text{reduce}_D(P)$ is accepted by an LTA.*

Interestingly, every reduction in $\text{reduce}_D(P)$ is optimal in the sense that each reduction contains at most one representative of each equivalence class of $\sim_D$.

Theorem 6.7. *Fix some $P \subseteq \Sigma^*$ and $R : \Sigma^* \to \mathcal{L}in(\Sigma)$. For all $(x, y) \in P \setminus \text{ignore}_R$, if $x \sim_D y$ then $x = y$.*

7 Algorithms

Figure 4 illustrates the outline of our verification algorithm. It is a counterexample-guided abstraction refinement loop in the style of [12, 13, 17]. The key difference is that instead of checking whether some proof Π is a proof for the program P, it checks if there exists a reduction of the program P that Π proves correct.

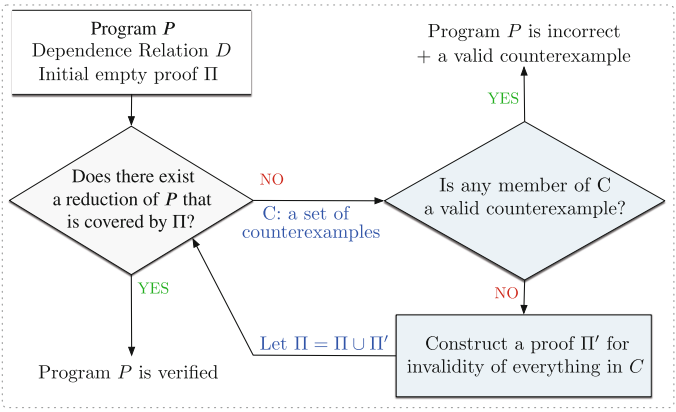

Fig. 4. Counterexample-guided refinement loop.

The algorithm relies on an oracle INTERPOLATE that, given a finite set of program traces C, returns a proof Π', if one exists, such that $C \subseteq \mathcal{L}(\Pi')$. In our tool, we use Craig interpolation to implement the oracle INTERPOLATE. In general, since program traces are the simplest form of sequential programs (loop and branch free), any automated program prover that can handle proving them may be used.

The results presented in Sects. 5 and 6 give rise to the proof checking sub routine of the algorithm in Fig. 4 (i.e. the light grey test). Given a program DFA $A_P = (Q_P, \Sigma, \delta_P, q_{P0}, F_P)$ and a proof DFA $A_\Pi = (Q_\Pi, \Sigma, \delta_\Pi, q_{\Pi 0}, F_\Pi)$ (obtained by determinizing Π_{NFA}), we can decide $\exists P' \in \text{reduce}_D(\mathcal{L}(A_P)). P' \subseteq \mathcal{L}(A_\Pi)$ by constructing an LTA $M_{P\Pi}$ for $\text{reduce}_D(\mathcal{L}(A_P)) \cap \mathcal{P}(\mathcal{L}(A_\Pi))$ and checking emptiness (Theorem 5.2).

7.1 Progress

The algorithm corresponding to Fig. 4 satisfies a weak progress theorem: none of the counterexamples from a round of the algorithm will ever appear in a

future counterexample set. This, however, is not strong enough to guarantee termination. Alternatively, one can think of the algorithm's progress as follows. In each round new assertions are discovered through the oracle INTERPOLATE, and one can optimistically hope that one can finally converge on an existing target proof Π^*. The success of this algorithm depends on two factors: (1) the counterexamples used by the algorithm belong to $\mathcal{L}(\Pi^*)$ and (2) the proof that INTERPOLATE discovers for these counterexamples coincide with Π^*. The latter is a typical known wild card in software model checking, which cannot be guaranteed; there is plenty of empirical evidence, however, that procedures based on Craig Interpolation do well in approximating it. The former is a new problem for our refinement loop.

In a standard algorithm in the style of [12,13,17], the verification proof rule dictates that every program trace must be in $\mathcal{L}(\Pi^*)$. In our setting, we only require a subset (corresponding to some reduction) to be in $\mathcal{L}(\Pi^*)$. This means one cannot simply rely on program traces as *appropriate* counterexamples. Theorem 5.4 presents a solution to this problem. It ensures that we always feed INTERPOLATE some counterexample from Π^* and therefore guarantee progress.

Theorem 7.1 (Strong Progress). *Assume a proof Π^* exists for some reduction $P^* \in \mathcal{R}$ and* INTERPOLATE *always returns some subset of Π^* for traces in $\mathcal{L}(\Pi^*)$. Then the algorithm will terminate in at most $|\Pi^*|$ iterations.*

Theorem 7.1 ensures that the algorithm will never get into an infinite loop due to a bad choice of counterexamples. The condition on INTERPOLATE ensures that divergence does not occur due to the wrong choice of assertions by INTERPOLATE and without it any standard interpolation-based software model checking algorithm may diverge. The assumption that there exists a proof for a reduction of the program in the fixed set $\mathcal{R}$ ensures that the proof checking procedure can verify the target proof Π^* once it is reached. Note that, in general, a proof may exist for a reduction of the program which is not in $\mathcal{R}$. Therefore, the algorithm is not complete with respect to all reductions, since checking the premises of SAFERED1 is undecidable as discussed in Sect. 4.

7.2 Faster Proof Checking Through Antichains

The state set of $M_{P\Pi}$, the intersection of program and proof LTAs, has size $|Q_P \times \mathbb{B} \times \mathcal{P}(\Sigma) \times Q_\Pi|$, which is exponential in $|\Sigma|$. Therefore, even a linear emptiness test for this LTA can be computationally expensive. Antichains have been previously used [8] to optimize certain operations over NFAs that also suffer from exponential blowups, such as deciding universality and inclusion tests. The main idea is that these operations involve computing downwards-closed and upwards-closed sets according to an appropriate subsumption relation, which can be represented compactly as antichains. We employ similar techniques to propose a new emptiness check algorithm.

Antichains. The set of maximal elements of a set X with respect to some ordering relation $\sqsubseteq$ is denoted $\max(X)$. The downwards-closure of a set X with

respect to $\sqsubseteq$ is denoted $\lfloor X \rfloor$. An antichain is a set X where no element of X is related (by $\sqsubseteq$) to another. The maximal elements $\max(X)$ of a finite set X is an antichain. If X is downwards-closed then $\lfloor \max(X) \rfloor = X$.

The emptiness check algorithm for LTAs from [2] computes the set of *inactive* states (i.e. states which generate an empty language) and checks if the initial state is inactive. The set of inactive states of an LTA $M = (Q, \Delta, q_0)$ is defined as the smallest set $\text{inactive}(M)$ satisfying

$$\frac{\forall (q, B, \sigma) \in \Delta.\, \exists a.\, \sigma(a) \in \text{inactive}(M)}{q \in \text{inactive}(M)} \qquad \text{(Inactive)}$$

Alternatively, one can view $\text{inactive}(M)$ as the least fixed-point of a monotone (with respect to $\subseteq$) function $F_M : \mathcal{P}(Q) \to \mathcal{P}(Q)$ where

$$F_M(X) = \{q \mid \forall (q, B, \sigma) \in \Delta.\, \exists a.\, \sigma(a) \in X\}.$$

Therefore, $\text{inactive}(M)$ can be computed using a standard fixpoint algorithm.

If $\text{inactive}(M)$ is downwards-closed with respect to some *subsumption relation* $(\sqsubseteq) \subseteq Q \times Q$, then we need not represent all of $\text{inactive}(M)$. The antichain $\max(\text{inactive}(M))$ of maximal elements of $\text{inactive}(M)$ (with respect to $\sqsubseteq$) would be sufficient to represent the entirety of $\text{inactive}(M)$, and can be exponentially smaller than $\text{inactive}(M)$, depending on the choice of relation $\sqsubseteq$.

A trivial way to compute $\max(\text{inactive}(M))$ is to first compute $\text{inactive}(M)$ and then find the maximal elements of the result, but this involves doing strictly more work than the baseline algorithm. However, observe that if F_M also preserves downwards-closedness with respect to $\sqsubseteq$, then

$$\begin{aligned} \max(\text{inactive}(M)) &= \max(\text{lfp}(F_M)) \\ &= \max(\text{lfp}(F_M \circ \lfloor - \rfloor \circ \max)) = \text{lfp}(\max \circ F_M \circ \lfloor - \rfloor) \end{aligned}$$

That is, $\max(\text{inactive}(M))$ is the least fixed-point of a function $F_M^{\max} : \mathcal{P}(Q) \to \mathcal{P}(Q)$ defined as $F_M^{\max}(X) = \max(F_M(\lfloor X \rfloor))$. We can calculate $\max(\text{inactive}(M))$ efficiently if we can calculate $F_M^{\max}(X)$ efficiently, which is true in the special case of the intersection automaton for the languages of our proof $\mathcal{P}(\mathcal{L}(\Pi))$ and our program $\text{reduce}_D(P)$, which we refer to as $M_{P\Pi}$.

We are most interested in the state space of $M_{P\Pi}$, which is $Q_{P\Pi} = (Q_P \times \mathbb{B} \times \mathcal{P}(\Sigma)) \times Q_\Pi$. Observe that states whose $\mathbb{B}$ part is $\top$ are always active:

Lemma 7.2. *$((q_P, \top, S), q_\Pi) \notin \text{inactive}(M_{P\Pi})$ for all $q_P \in Q_P$, $q_\Pi \in Q_\Pi$, and $S \subseteq \Sigma$.*

The state space can then be assumed to be $Q_{P\Pi} = (Q_P \times \{\bot\} \times \mathcal{P}(\Sigma)) \times Q_\Pi$ for the purposes of checking inactivity. The subsumption relation defined as the smallest relation $\sqsubseteq_{P\Pi}$ satisfying

$$S \subseteq S' \implies ((q_P, \bot, S), q_\Pi) \sqsubseteq_{P\Pi} ((q_P, \bot, S'), q_\Pi)$$

for all $q_P \in Q_P$, $q_\Pi \in Q_\Pi$, and $S, S' \subseteq \Sigma$, is a suitable one since:

Lemma 7.3. *$F_{M_{P\Pi}}$ preserves downwards-closedness with respect to $\sqsubseteq_{P\Pi}$.*

The function $F^{\max}_{M_{P\Pi}}$ is a function over relations

$$F^{\max}_{M_{P\Pi}} : \mathcal{P}((Q_P \times \{\bot\} \times \mathcal{P}(\Sigma)) \times Q_\Pi) \to \mathcal{P}((Q_P \times \{\bot\} \times \mathcal{P}(\Sigma)) \times Q_\Pi)$$

but in our case it is more convenient to view it as a function over functions

$$F^{\max}_{M_{P\Pi}} : (Q_P \times \{\bot\} \times Q_\Pi \to \mathcal{P}(\mathcal{P}(\Sigma))) \to (Q_P \times \{\bot\} \times Q_\Pi \to \mathcal{P}(\mathcal{P}(\Sigma)))$$

Through some algebraic manipulation and some simple observations, we can define $F^{\max}_{M_{P\Pi}}$ functionally as follows.

Lemma 7.4. *For all $q_P \in Q_P$, $q_\Pi \in Q_\Pi$, and $X : Q_P \times \{\bot\} \times Q_\Pi \to \mathcal{P}(\mathcal{P}(\Sigma))$,*

$$F^{\max}_{M_{P\Pi}}(X)(q_P, \bot, q_\Pi) = \begin{cases} \{\Sigma\} & \text{if } q_P \in F_P \wedge q_\Pi \notin F_\Pi \\ \bigsqcap_{R \in \mathcal{L}in(\Sigma)} \bigsqcup_{\substack{a \in \Sigma \\ S \in X(q'_P, \bot, q'_\Pi)}} S' & \text{otherwise} \end{cases}$$

where

$$q'_P = \delta_P(q_P, a) \qquad X \sqcap Y = \max\{x \cap y \mid x \in X \wedge y \in Y\}$$
$$q'_\Pi = \delta_\Pi(q_\Pi, a) \qquad X \sqcup Y = \max(X \cup Y)$$

$$S' = \begin{cases} \{(S \cup D(a)) \setminus \{a\}\} & \text{if } R(a) \setminus D(a) \subseteq S \\ \emptyset & \text{otherwise} \end{cases}$$

```
function Check(A_P, A_Π, D)
    (Q_P, Σ, δ_P, q_0P, F_P) ← A_P
    (Q_Π, Σ, δ_Π, q_0Π, F_Π) ← A_Π
    function FMax(X)((q_P, ⊥, q_Π))
        if q_P ∈ F_P ∧ q_Π ∉ F_Π
            return {Σ}
        X^⊓ ← {Σ}
        for R ∈ Lin(Σ)
            X^⊔ ← ∅
            for a ∈ Σ, S ∈ X((δ_P(q_P, a), ⊥, δ_Π(q_Π, a)))
                if R(a) \ D(a) ⊆ S
                    X^⊔ ← X^⊔ ⊔ {(S ∪ D(a)) \ {a}}
            X^⊓ ← X^⊓ ⊓ X^⊔
        return X^⊓
    return Fix(FMax)((q_0P, ⊥, q_0Π)) ≠ ∅
```

Algorithm 1. Proof checking algorithm

A full justification appears in [14]. Formulating $F^{\max}_{M_{P\Pi}}$ as a higher-order function allows us to calculate $\max(\text{inactive}(M_{P\Pi}))$ using efficient fixpoint algorithms like the one in [22]. Algorithm 1 outlines our proof checking routine. $\textsc{Fix} : ((A \to B) \to (A \to B)) \to (A \to B)$ is a procedure that computes the least fixpoint of its input. The algorithm simply computes the fixpoint of the function $F^{\max}_{M_{P\Pi}}$ as defined in Lemma 7.4, which is a compact representation of $\text{inactive}(M_{P\Pi})$ and checks if the start state of $M_{P\Pi}$ is in it.

Counterexamples. Theorem 5.4 states that a finite set of counterexamples exists whenever $\exists P' \in \text{reduce}_D(P).\, P' \subseteq \mathcal{L}(\Pi)$ does not hold. The proof of emptiness for an LTA, formed using rule INACTIVE above, is a finite tree. Each edge in the tree is labelled by an element of Σ (obtained from the existential in the rule) and the paths through this tree form the counterexample set. To compute this set, then, it suffices to remember enough information during the computation of $\text{inactive}(M)$ to reconstruct the proof tree. Every time a state q is determined to be inactive, we must also record the witness $a \in \Sigma$ for each transition $(q, B, \sigma) \in \Delta$ such that $\sigma(a) \in \text{inactive}(M)$.

In an antichain-based algorithm, once we determine a state q to be inactive, we simultaneously determine everything it subsumes (i.e. $\sqsubseteq q$) to be inactive as well. If we record unique witnesses for each and every state that q subsumes, then the space complexity of our antichain algorithm will be the same as the unoptimized version. The following lemma states that it is sufficient to record witnesses only for q and discard witnesses for states that q subsumes.

Lemma 7.5. *Fix some states q, q' such that $q' \sqsubseteq_{P\Pi} q$. A witness used to prove q is inactive can also be used to prove q' is inactive.*

Note that this means that the antichain algorithm soundly returns potentially fewer counterexamples than the original one.

7.3 Partition Optimization

The LTA construction for $\text{reduce}_D(P)$ involves a nondeterministic choice of linear order at each state. Since $|\mathcal{L}in(\Sigma)|$ has size $|\Sigma|!$, each state in the automaton would have a large number of transitions. As an optimization, our algorithm selects ordering relations out of $\mathcal{P}art(\Sigma)$ (instead of $\mathcal{L}in(\Sigma)$), defined as $\mathcal{P}art(\Sigma) = \{\Sigma_1 \times \Sigma_2 \mid \Sigma_1 \uplus \Sigma_2 = \Sigma\}$ where $\uplus$ is disjoint union. This leads to a sound algorithm which is not complete with respect to sleep set reductions and trades the factorial complexity of computing $\mathcal{L}in(\Sigma)$ for an exponential one.

8 Experimental Results

To evaluate our approach, we have implemented our algorithm in a tool called WEAVER written in Haskell. WEAVER accepts a program written in a simple imperative language as input, where the property is already encoded in the program in the form of *assume* statements, and attempts to prove the program

correct. The dependence relation for each input program is computed using a heuristic that ensures $\sim_D$-closedness. It is based on the fact that the shuffle product (i.e. parallel composition) of two $\sim_D$-closed languages is $\sim_D$-closed.

Weaver employs two verification algorithms: (1) The total order algorithm presented in Algorithm 1, and (2) the variation with the partition optimization discussed in Sect. 7.3. It also implements multiple counterexample generation algorithms: (1) *Naive:* selects the first counterexample in the difference of the program and proof language. (2) *Progress-Ensuring:* selects a set of counterexamples satisfying Theorem 5.4. (3) *Bounded Progress-Ensuring:* selects a few counterexamples (in most cases just one) from the set computed by the progress-ensuring algorithm. Our experimentation demonstrated that in the vast majority of the cases, the bounded progress ensuring algorithm (an instance of the partition algorithm) is the fastest of all options. Therefore, all our reports in this section are using this instance of the algorithm.

For the larger benchmarks, we use a simple sound optimization to reduce the proof size. We declare the basic blocks of code as atomic, so that internal assertions need not be generated for them as part of the proof. This optimization is incomplete with respect to sleep set reductions.

Benchmarks. We use a set of sequential benchmarks from [24] and include additional sequential benchmarks that involve more interesting reductions in their proofs. We have a set of parallel benchmarks, which are beyond the scope of previous hypersafety verification techniques. We use these benchmarks to demonstrate that our technique/tool can seamlessly handle concurrency. These involve proving concurrency specific hypersafety properties such as determinism and equivalence of parallel and sequential implementations of algorithms. Finally, since the proof checking algorithm is the core contribution of this paper, we have a contrived set of instances to stress test our algorithm. These involve proving determinism of simple parallel-disjoint programs with various numbers of threads and statements per thread. These benchmarks have been designed to cause a combinatorial explosion for the proof checker and counterexample generation routines. More information on the benchmarks can be found in [14].

Evaluation

Due to space restrictions, it is not feasible to include a detailed account of all our experiments here, for over 50 benchmarks. A detailed table can be found in [14]. Table 1 includes a summary in the form of averages, and here, we discuss our top findings.

Proof construction time refers to the time spent to construct $\mathcal{L}(\Pi)$ from a given set of assertions Π and excludes the time to produce proofs for the counterexamples in a given round. **Proof checking time** is the time spent to check if the current proof candidate is strong enough for a reduction of the program. In the fastest instances (total time around 0.01 s), roughly equal time is spent in proof checking and proof construction. In the slowest instances, the total time is almost entirely spent in proof construction. In contrast, in our stress

Table 1. Experimental results averages for benchmark groups.

Benchmark group	Group count	Proof size	Number of refinement rounds	Proof construction time	Proof checking time	Total time
Looping programs of [24] 2-safety properties	5	63	12	46.69 s	0.1 s	47.03 s
Looping programs of [24] 3-safety properties	8	155	22	475.78 s	11.79 s	448.36 s
Loop-free programs of [24]	27	5	2	0.13 s	0.0004 s	0.15 s
Our sequential benchmarks	13	30	9	14.27 s	2.5 s	17.94 s
Our parallel benchmarks	7	31	8	17.95	0.56 s	18.63 s

tests (designed to stress the proof checking algorithm) the majority of the time is spent in proof checking. The time spent in proving counterexamples correct is negligible in all instances. **Proof sizes** vary from 4 assertions to 298 for the most complicated instance. Verification times are *correlated* with the final proof size; larger proofs tend to cause longer verification times.

Numbers of refinement rounds vary from 2 for the simplest to 33 for the most complicated instance. A small number of refinement rounds (e.g. 2) implies a fast verification time. But, for the higher number of rounds, a strong positive correlation between the number of rounds and verification time does not exist.

For our **parallel programs** benchmarks (other than our stress tests), the tool spends the majority of its time in proof construction. Therefore, we designed specific (unusual) parallel programs to stress test the proof checker. **Stress test** benchmarks are trivial tests of determinism of disjoint parallel programs, which can be proven correct easily by using the atomic block optimization. However, we force the tool to do the unnecessary hard work. These instances simulate the worst case theoretical complexity where the proof checking time and number of counterexamples grow exponentially with the number of threads and the sizes of the threads. In the largest instance, more than 99% of the total verification time is spent in proof checking. Averages are not very informative for these instances, and therefore are not included in Table 1.

Finally, Weaver is only slow for verifying 3-safety properties of large looping benchmarks from [24]. Note that unlike the approach in [24], which starts from a default lockstep reduction (that is incidentally sufficient to prove these instances), we do not assume any reduction and consider them all. The extra time is therefore expected when the product programs become quite large.

9 Related Work

The notion of a k-safety hyperproperty was introduced in [7] without consideration for automatic program verification. The approach of reducing k-safety to 1-safety by self-composition is introduced in [5]. While theoretically complete, self-composition is not practical as discussed in Sect. 1. Product programs generalize the self-composition approach and have been used in verifying translation

validation [20], non-interference [16,23], and program optimization [25]. A product of two programs P_1 and P_2 is semantically equivalent to $P_1 \cdot P_2$ (sequential composition), but is made easier to verify by allowing parts of each program to be interleaved. The product programs proposed in [3] allow lockstep interleaving exclusively, but only when the control structures of P_1 and P_2 match. This restriction is lifted in [4] to allow some non-lockstep interleavings. However, the given construction rules are non-deterministic, and the choice of product program is left to the user or a heuristic.

Relational program logics [6,28] extend traditional program logics to allow reasoning about relational program properties, however automation is usually not addressed. Automatic construction of product programs is discussed in [10] with the goal of supporting procedure specifications and modular reasoning, but is also restricted to lockstep interleavings. Our approach does not support procedure calls but is fully automated and permits non-lockstep interleavings.

The key feature of our approached is the automation of the discovery of an appropriate program reduction and a proof combined. In this case, the only other method that compares is the one based on Cartesian Hoare Logic (CHL) proposed in [24] along with an algorithm for automatic verification based on CHL. Their proposed algorithm implicitly constructs a product program, using a heuristic that favours lockstep executions as much as possible, and then prioritizes certain rules of the logic over the rest. The heuristic nature of the search for the proof means that no characterization of the search space can be given, and no guarantees about whether an appropriate product program will be found. In contrast, we have a formal characterization of the set of explored product programs in this paper. Moreover, CHL was not designed to deal with concurrency.

Lipton [19] first proposed reduction as a way to simplify reasoning about concurrent programs. His ideas have been employed in a semi-automatic setting in [11]. Partial-order reduction (POR) is a class of techniques that reduces the state space of search by removing redundant paths. POR techniques are concerned with finding a single (preferably minimal) reduction of the input program. In contrast, we use the same underlying ideas to explore many program reductions simultaneously. The class of reductions described in Sect. 6 is based on the sleep set technique of Godefroid [15]. Other techniques exist [1,15] that are used in conjunction with sleep sets to achieve minimality in a normal POR setting. In our setting, reductions generated by sleep sets are already optimal (Theorem 6.7). However, employing these additional POR techniques may propose ways of optimizing our proof checking algorithm by producing a smaller reduction LTA.

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