Automata Terms in a Lazy WSkS Decision Procedure (Technical Report)

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Abstract. We propose a lazy decision procedure for the logic WSkS. It builds a term-based symbolic representation of the state space of the tree automaton (TA) constructed by the classical WSkS decision procedure. The classical decision procedure transforms the symbolic representation into a TA via a bottom-up traversal and then tests its language non-emptiness, which corresponds to satisfiability of the formula. On the other hand, we start evaluating the representation from the top, construct the state space on the fly, and utilize opportunities to prune away parts of the state space irrelevant to the language emptiness test. In order to do so, we needed to extend the notion of *language terms* (denoting language derivatives) used in our previous procedure for the linear fragment of the logic (the so-called WS1S) into *automata terms*. We implemented our decision procedure and identified classes of formulae on which our prototype implementation is significantly faster than the classical procedure implemented in the Mona tool.

1 Introduction

Weak monadic second-order logic of k successors (WSkS) is a logic for describing regular properties of finite k-ary trees. In addition to talking about trees, WSkS can also encode complex properties of a rich class of general graphs by referring to their tree backbones [1]. WSkS offers extreme succinctness for the price of non-elementary worst-case complexity. As noticed first by the authors of [2] in the context of WS1S (a restriction that speaks about finite words only), the trade-off between complexity and succinctness may, however, be turned significantly favourable in many practical cases through a use of clever implementation techniques and heuristics. Such techniques were then elaborated in the tool Mona [3,4], the best-known implementation of decision procedures for WS1S and WS2S. Mona has found numerous applications in verification of programs with complex dynamic linked data structures [1,5,6,7,8], string programs [9], array programs [10], parametric systems [11,12,13], distributed systems [14,15], hardware verification [16], automated synthesis [17,18,19], and even computational linguistics [20].

Despite the extensive research and engineering effort invested into Mona, due to which it still offers the best all-around performance among existing WS1S/WS2S decision procedures, it is, however, easy to reach its scalability limits. Particularly, Mona implements the classical WS1S/WS2S decision procedures that build a word/tree automaton representing models of the given formula and then check emptiness of the automaton's language. The non-elementary complexity manifests in that the size of the automaton is prone to explode, which is caused mainly by the repeated determinisation

(needed to handle negation and alternation of quantifiers) and synchronous product construction (used to handle conjunctions and disjunctions). Users of WSkS are then forced to either find workarounds, such as in [6], or, often restricting the input of their approach, give up using WSkS altogether [21].

As in Mona, we further consider WS2S only (this does not change the expressive power of the logic since *k*-ary trees can be easily encoded into binary ones). We revisit the use of tree automata (TAs) in the WS2S decision procedure and obtain a new decision procedure that is much more efficient in certain cases. It is inspired by works on *antichain algorithms* for efficient testing of universality and language inclusion of finite automata [22,23,24,25], which implement the operations of testing emptiness of a complement (universality) or emptiness of a product of one automaton with the complement of the other one (language inclusion) via an *on-the-fly* determinisation and product construction. The on-the-fly approach allows one to achieve significant savings by pruning the state space that is irrelevant for the language emptiness test. The pruning is achieved by early termination when detecting non-emptiness (which represents a simple form of *lazy evaluation*), and *subsumption* (which basically allows one to disregard proof obligations that are implied by other ones). Antichain algorithms and their generalizations have shown great efficiency improvements in applications such as abstract regular model checking [24], shape analysis [26], LTL model checking [27], or game solving [28].

Our work generalizes the above mentioned approaches of on-the-fly automata construction, subsumption, and lazy evaluation for the needs of deciding WS2S. In our procedure, the TAs that are constructed explicitly by the classical procedure are represented symbolically by the so-called *automata terms*. More precisely, we build automata terms for subformulae that start with a quantifier (and for the top-level formula) only—unlike the classical procedure, which builds a TA for every subformula. Intuitively, automata terms specify the set of leaf states of the TAs of the appropriate (sub)formulae. The leaf states themselves are then represented by *state terms*, whose structure records the automata constructions (corresponding to Boolean operations and quantification on the formula level) used to create the given TAs from base TAs corresponding to atomic formulae. The leaves of the terms correspond to states of the base automata. Automata terms may be used as state terms over which further automata terms of an even higher level are built. Non-leaf states, the transition relation, and root states are then given implicitly by the transition relations of the base automata and the structure of the state terms.

Our approach is a generalization of our earlier work [29] on WS1S. Although the term structure and the generalized algorithm may seem close to [29], the reasoning behind it is significantly more involved. Particularly, [29] is based on defining the semantics (language) of terms as a function of the semantics of their sub-terms. For instance, the semantics of the term $\{q_1, \ldots, q_n\}$ is defined as the union of languages of the state terms q_1, \ldots, q_n , where the language of a state of the base automaton consists of the words accepted at that state. With TAs, it is, however, not meaningful to talk about trees accepted from a leaf state, instead, we need to talk about a given state and its context, i.e., other states that could be obtained via a bottom-up traversal over the given set of symbols. Indeed, trees have multiple leafs, which may be accepted by a number of different states, and so a tree is accepted from a set of states, not from any single one of them alone. We therefore cannot define the semantics of a state term as a tree language,

and so we cannot define the semantics of an automata term as the union of the languages of its state sub-terms. This problem seems critical at first because without a sensible notion of the meaning of terms, a straightforward generalization of the algorithm of [29] to trees does not seem possible. The solution we present here is based on defining the semantics of terms via the automata constructions they represent rather then as functions of languages of their sub-terms.

Unlike the classical decision procedure, which builds a TA corresponding to a formula bottom-up, i.e. from the atomic formulae, we build automata terms top-down, i.e., from the top-level formula. This approach offers a lot of space for various optimisations. Most importantly, we test non-emptiness of the terms on the fly during their construction and construct the terms lazily. In particular, we use short-circuiting for dealing with the \land and \lor connectives and early termination with possible continuation when implementing the fixpoint computations needed when dealing with quantifiers. That is, we terminate the fixpoint computation whenever the emptiness can be decided in the given computation context and continue with the computation when such a need appears once the context is changed on some higher-term level. Further, we define a notion of subsumption of terms, which, intuitively, compares the terms wrt the sets of trees they represent, and allows us to discard terms that are subsumed by others.

We have implemented our approach in a prototype tool. When experimenting with it, we have identified multiple parametric families of WS2S formulae where our implementation can—despite its prototypical form—significantly outperform Mona. We find this encouraging since there is a lot of space for further optimisations and, moreover, our implementation can be easily combined with Mona by treating automata constructed by Mona in the same way as if they were obtained from atomic predicates.

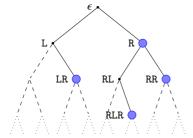
This is an extended version of the paper [30].

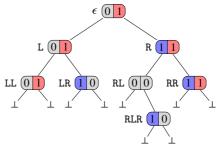
2 Preliminaries

In this section, we introduce basic notation, trees, and tree automata, and give a quick introduction to the *weak monadic second-order logic of two successors* (WS2S) and its classical decision procedure. We give the minimal syntax of WS2S only; see, e.g., Comon *et al.* [31] for more details.

Basics, Trees, and Tree Automata. Let Σ be a finite set of symbols, called an *alphabet*. The set Σ^* of *words* over Σ consists of finite sequences of symbols from Σ . The *empty word* is denoted by ϵ , with $\epsilon \notin \Sigma$. The *concatenation* of two words ϵ and ϵ is denoted by ϵ words is denoted by ϵ . The *domain* of a partial function ϵ is the set ϵ and ϵ is the set ϵ and its ϵ is the set ϵ is the function ϵ is the set ϵ in ϵ in ϵ in ϵ is the function ϵ in ϵ in

We will consider ordered binary trees. We call a word $p \in \{L, R\}^*$ a tree *position* and p.L and p.R its *left* and *right child*, respectively. Given an alphabet Σ s.t. $\bot \notin \Sigma$, a *tree* over Σ is a finite partial function $\tau: \{L, R\}^* \to (\Sigma \cup \{\bot\})$ such that (i) $\operatorname{dom}(\tau)$ is non-empty and prefix-closed, and (ii) for all positions $p \in \operatorname{dom}(t)$, either $\tau(p) \in \Sigma$ and p has both children, or $\tau(p) = \bot$ and p has no children, in which case it is called





- (a) Positions assigned to the variable *X*.
- (b) Encoding of ν into a tree τ_{ν} ; a node at a position p has the value $(x \mid y)$ where x = 1 iff $\tau_{\nu}(p)$ maps X to 1 and y = 1 iff $\tau_{\nu}(p)$ maps Y to 1.

Fig. 1: An example of an assignment ν to a pair of variables $\{X,Y\}$ s.t. $\nu(X) = \{LR, R, RLR, RR\}$ and $\nu(Y) = \{\epsilon, L, LL, R, RR\}$ and its encoding into a tree.

a *leaf*. We let $leaf(\tau)$ be the set of all leaves of τ . The position ϵ is called the *root*, and we write Σ^{\pm} to denote the set of all trees over Σ^{1} . We abbreviate $\{a\}^{\pm}$ as a^{\pm} for $a \in \Sigma$.

The *sub-tree* of τ rooted at a position $p \in \operatorname{dom}(\tau)$ is the tree $\tau' = \{p' \mapsto \tau(p.p') \mid p.p' \in \operatorname{dom}(\tau)\}$. A *prefix* of τ is a tree τ' such that $\tau'_{|\operatorname{dom}(\tau')\setminus leaf(\tau')|} \subseteq \tau_{|\operatorname{dom}(\tau)\setminus leaf(\tau)|}$. The *derivative* of a tree τ wrt a set of trees $S \subseteq \Sigma^{\pm}$ is the set $\tau - S$ of all prefixes τ' of τ such that, for each position $p \in leaf(\tau')$, the sub-tree of τ at p either belongs to S or it is a leaf of τ . Intuitively, $\tau - S$ are all prefixes of τ obtained from τ by removing some of the sub-trees in S. The derivative of a set of trees $T \subseteq \Sigma^{\pm}$ wrt S is the set $\bigcup_{\tau \in T} (\tau - S)$.

A (binary) tree automaton (TA) over an alphabet Σ is a quadruple $\mathcal{A} = (Q, \delta, I, R)$ where Q is a finite set of states, $\delta: Q^2 \times \Sigma \to 2^Q$ is a transition function, $I \subseteq Q$ is a set of leaf states, and $R \subseteq Q$ is a set of root states. We use (q,r)-(a)-s to denote that $s \in \delta((q,r),a)$. A run of \mathcal{A} on a tree τ is a total map $\rho: \mathrm{dom}(\tau) \to Q$ such that if $\tau(p) = \bot$, then $\rho(p) \in I$, else $(\rho(p.\mathbb{L}), \rho(p.\mathbb{R}))$ -(a)- $\rho(p)$ with $a = \tau(p)$. The run ρ is accepting if $\rho(\epsilon) \in R$, and the language $\mathcal{L}(\mathcal{A})$ of \mathcal{A} is the set of all trees on which \mathcal{A} has an accepting run. \mathcal{A} is deterministic if |I| = 1 and $\forall q, r \in Q, a \in \Sigma: |\delta((q,r),a)| \le 1$, and complete if $I \ge 1$ and $\forall q, r \in Q, a \in \Sigma: |\delta((q,r),a)| \ge 1$. Last, for $a \in \Sigma$, we shorten $\delta((q,r),a)$ as $\delta_a(q,r)$, and we use $\delta_{\Gamma}(q,r)$ to denote $\bigcup \{\delta_a(q,r) \mid a \in \Gamma\}$ for a set $\Gamma \subseteq \Sigma$.

Syntax and Semantics of WS2S. WS2S is a logic that allows quantification over second-order *variables*, which are denoted by upper-case letters X, Y, \ldots and range over *finite sets* of tree positions in $\{L, R\}^*$ (the finiteness of variable assignments is reflected in the name *weak*). See Fig. 1a for an example of a set of positions assigned to a variable. Atomic formulae (atoms) of WS2S are of the form: (i) $X \subseteq Y$, (ii) $X = S_L(Y)$, and (iii) $X = S_R(Y)$. Formulae are constructed from atoms using the logical connectives A, \neg , and the quantifier A where A is a finite set of variables (we write A when A

¹ Intuitively, the $[\cdot]^{\bigstar}$ operator can be seen as a generalization of the Kleene star to tree languages. The symbol \bigstar is the Chinese character for a tree, pronounced $m\mathring{u}$, as in English moo-n, but shorter and with a falling tone, staccato-like.

is a singleton set $\{X\}$). Other connectives (such as \vee or \forall) and predicates (such as the predicate $\operatorname{Sing}(X)$ for a singleton set X) can be obtained as syntactic sugar (see App. B).

A model of a WS2S formula $\varphi(\mathbb{X})$ with the set of free variables \mathbb{X} is an assignment $\nu: \mathbb{X} \to 2^{\{L,R\}^*}$ of the free variables of φ to finite subsets of $\{L,R\}^*$ for which the formula is satisfied, written $\nu \models \varphi$. Satisfaction of atomic formulae is defined as follows: (i) $\nu \models X \subseteq Y$ iff $\nu(X) \subseteq \nu(Y)$, (ii) $\nu \models X = S_L(Y)$ iff $\nu(X) = \{p.L \mid p \in \nu(Y)\}$, and (iii) $\nu \models X = S_R(Y)$ iff $\nu(X) = \{p.R \mid p \in \nu(Y)\}$. Informally, the $S_L(Y)$ function returns all positions from Y shifted to their left child and the $S_R(Y)$ function returns all positions from Y shifted to their right child. Satisfaction of formulae built using Boolean connectives and the quantifier is defined as usual. A formula φ is valid, written $\models \varphi$, iff all assignments of its free variables are its models, and satisfiable if it has a model. Wlog, we assume that each variable in a formula either has only free occurrences or is quantified exactly once; we denote the set of (free and quantified) variables occurring in a formula φ as $Vars(\varphi)$.

Representing Models as Trees. We fix a formula φ with variables $Vars(\varphi) = \mathbb{X}$. A *symbol* ξ over \mathbb{X} is a (total) function $\xi : \mathbb{X} \to \{0,1\}$, e.g., $\xi = \{X \mapsto 0, Y \mapsto 1\}$ is a symbol over $\mathbb{X} = \{X,Y\}$. We use $\Sigma_{\mathbb{X}}$ to denote the set of all symbols over \mathbb{X} and 0 to denote the symbol mapping all variables in \mathbb{X} to 0, i.e., $\vec{0} = \{X \mapsto 0 \mid X \in \mathbb{X}\}$.

A finite assignment $\nu: \mathbb{X} \to 2^{\{\mathrm{L},\mathrm{R}\}^*}$ of φ 's variables can be encoded as a finite tree τ_{ν} of symbols over \mathbb{X} where every position $p \in \{\mathrm{L},\mathrm{R}\}^*$ satisfies the following conditions: (a) if $p \in \nu(X)$, then $\tau_{\nu}(p)$ contains $\{X \mapsto 1\}$, and (b) if $p \notin \nu(X)$, then either $\tau_{\nu}(p)$ contains $\{X \mapsto 0\}$ or $\tau_{\nu}(p) = \bot$ (note that the occurrences of \bot in τ are limited since τ still needs to be a tree). Observe that ν can have multiple encodings: the unique minimum one τ_{ν}^{min} and (infinitely many) extensions of τ_{ν}^{min} with $\vec{0}$ -only trees. The language of φ is defined as the set of all encodings of its models $\mathcal{L}(\varphi) = \{\tau_{\nu} \in \Sigma_{\mathbb{X}}^{\star} \mid \nu \models \varphi \text{ and } \tau_{\nu} \text{ is an encoding of } \nu\}$.

Let ξ be a symbol over \mathbb{X} . For a set of variables $\mathbb{Y} \subseteq \mathbb{X}$, we define the *projection* of ξ wrt \mathbb{Y} as the set of symbols $\pi_{\mathbb{Y}}(\xi) = \{\xi' \in \Sigma_{\mathbb{X}} \mid \xi_{|\mathbb{X} \setminus \mathbb{Y}} \subseteq \xi'\}$. Intuitively, the projection removes the original assignments of variables from \mathbb{Y} and allows them to be substituted by any possible value. We define $\pi_{\mathbb{Y}}(\bot) = \bot$ and write π_{Y} if \mathbb{Y} is a singleton set $\{Y\}$. As an example, for $\mathbb{X} = \{X,Y\}$ the projection of $\vec{0}$ wrt $\{X\}$ is given as $\pi_{X}(\vec{0}) = \{\{X \mapsto 0, Y \mapsto 0\}, \{X \mapsto 1, Y \mapsto 0\}\}$. The definition of projection can be extended to trees τ over $\Sigma_{\mathbb{X}}$ so that $\pi_{\mathbb{Y}}(\tau)$ is the set of trees $\{\tau' \in \Sigma_{\mathbb{X}}^{\pm} \mid \forall p \in \mathrm{pos}(\tau) : \mathrm{if} \ \tau(p) = \bot$, then $\tau'(p) = \bot$, else $\tau'(p) \in \pi_{\mathbb{Y}}(\tau(p))$ and subsequently to languages L so that $\pi_{\mathbb{Y}}(L) = \bigcup \{\pi_{\mathbb{Y}}(\tau) \mid \tau \in L\}$.

The Classical Decision Procedure for WS2S. The classical decision procedure for the WS2S logic goes through a direct construction of a TA \mathcal{A}_{φ} having the same language as a given formula φ . Let us briefly recall the automata constructions used (cf. [31]). Given a complete TA $\mathcal{A} = (Q, \delta, I, R)$, the *complement* assumes that \mathcal{A} is deterministic and returns $\overline{\mathcal{A}} = (Q, \delta, I, Q \setminus R)$, the projection returns $\pi_X(\mathcal{A}) = (Q, \delta^{\pi_X}, I, R)$

² Note that our definition of projection differs from the usual one, which would in the example produce a single symbol $\{Y \mapsto 0\}$ over a different alphabet (the alphabet of symbols over $\{Y\}$).

with $\delta_a^{\pi_X}(q,r) = \delta_{\pi_X(a)}(q,r)$, and the *subset construction* returns the deterministic and complete automaton $\mathcal{A}^{\mathcal{D}} = \{2^Q, \delta^{\mathcal{D}}, \{I\}, R^{\mathcal{D}}\}$ where $\delta_a^{\mathcal{D}}(S,S') = \bigcup_{q \in S, q' \in S'} \delta_a(q,q')$ and $R^{\mathcal{D}} = \{S \subseteq Q \mid S \cap R \neq \emptyset\}$. The binary operators $\circ \in \{\cup, \cap\}$ are implemented through a *product construction*, which—given the TA \mathcal{A} and another complete TA $\mathcal{A}' = (Q', \delta', I', R')$ —returns the automaton $\mathcal{A} \circ \mathcal{A}' = (Q \times Q', \Delta^{\times}, I^{\times}, R^{\circ})$ where $\Delta_a^{\times}((q,r),(q',r')) = \Delta_a(q,q') \times \Delta_a'(r,r')$, $I^{\times} = I \times I'$, and for $(q,r) \in Q \times Q'$, $(q,r) \in R^{\cap} \Leftrightarrow q \in R \land r \in R'$ and $(q,r) \in R^{\cup} \Leftrightarrow q \in R \lor r \in R'$. The language non-emptiness test can be implemented through the equivalence $\mathcal{L}(\mathcal{A}) \neq \emptyset$ iff $reach_{\delta}(I) \cap R \neq \emptyset$ where the set $reach_{\delta}(S)$ of states reachable from a set $S \subseteq Q$ through δ -transitions is computed as the least fixpoint

$$reach_{\delta}(S) = \mu Z. \ S \cup \bigcup_{q,r \in Z} \delta(q,r).$$
 (1)

The same fixpoint computation is used to compute the derivative wrt a^{\dagger} for some $a \in \Sigma$ as $\mathcal{A} - a^{\dagger} = (Q, \delta, reach_{\delta_a}(I), R)$: the new leaf states are all those reachable from I through a-transitions.

The classical WSkS decision procedure uses the above operations to constructs the automaton \mathcal{A}_{φ} inductively to the structure of φ as follows: (i) If φ is an atomic formula, then \mathcal{A}_{φ} is a pre-defined *base* TA over $\Sigma_{\mathbb{X}}$ (the particular base automata for our atomic predicates can be found, e.g., in [31], and we list them also in App. C). (ii) If $\varphi = \varphi_1 \wedge \varphi_2$, then $\mathcal{A}_{\varphi} = \overline{\mathcal{A}_{\varphi_1}} \cap \mathcal{A}_{\varphi_2}$. (iii) If $\varphi = \varphi_1 \vee \varphi_2$, then $\mathcal{A}_{\varphi} = \mathcal{A}_{\varphi_1} \cup \mathcal{A}_{\varphi_2}$. (iv) If $\varphi = \neg \psi$, then $\mathcal{A}_{\varphi} = \overline{\mathcal{A}_{\psi}}$. (v) Finally, if $\varphi = \exists X. \ \psi$, then $\mathcal{A}_{\varphi} = (\pi_X(\mathcal{A}_{\psi}))^{\mathcal{D}} - \vec{0}^{\star}$.

Points (i) to (iv) are self-explanatory. In point (v), the projection implements the quantification by forgetting the values of the X component of all symbols. Since this yields non-determinism, projection is followed by determinisation by the subset construction. Further, the projection can produce some new trees that contain $\vec{0}$ -only labelled sub-trees, which need not be present in some smaller encodings of the same model. Consider, for example, a formula ψ having the language $\mathcal{L}(\psi)$ given by the tree τ_{ν} in Fig. 1b and all its $\vec{0}$ -extensions. To obtain $\mathcal{L}(\exists X.\psi)$, it is not sufficient to make the projection $\pi_X(\mathcal{L}(\psi))$ because the projected language does not contain the minimum encoding τ_{ν}^{min} of $\nu: Y \mapsto \{\epsilon, L, LL, R, RR\}$, but only those encodings ν' such that $\nu'(RLR) = \{Y \mapsto 0\}$. Therefore, the $\vec{0}$ -derivative is needed to saturate the language with all encodings of the encoded models (if some of these encodings were missing, the inductive construction could produce a wrong result, for instance, if the language were subsequently complemented). Note that the same effect can be achieved by replacing the set of leaf states I of \mathcal{A}_{φ} by $reach_{\Delta_{\vec{0}}}(I)$ where Δ is the transition function of \mathcal{A}_{φ} . See [31] for more details.

3 Automata Terms

Our algorithm for deciding WS2S may be seen as an alternative implementation of the classical procedure from Section 2. The main innovation is the data structure of *automata terms*, which implicitly represent the automata constructed by the automata operations. Unlike the classical procedure—which proceeds by a bottom-up traversal on the formula structure, building an automaton for each sub-formula before proceeding

upwards—automata terms allow for constructing parts of automata at higher levels from parts of automata on the lower levels even though the construction of the lower level automata has not yet finished. This allows one to test the language emptiness on the fly and use techniques of state space pruning, which will be discussed later in Section 4. Proofs of the lemmas can be found in App. A.

Syntax of automata terms. Terms are created according to the grammar in Fig. 2 starting from states $q \in Q_i$, denoted as *atomic states*, of a given finite set of *base automata* $\mathcal{B}_i = (Q_i, \delta_i, I_i, R_i)$ with pairwise disjoint sets of states. For simplicity, we assume that the base automata are complete, and we denote by $\mathcal{B} = (Q^{\mathcal{B}}, \delta^{\mathcal{B}}, I^{\mathcal{B}}, R^{\mathcal{B}})$ their component-wise

$$A ::= S \mid D \qquad (automata\ term)$$

$$S ::= \{t, \dots, t\} \qquad (set\ term)$$

$$D ::= S - \vec{0}^{*} \qquad (derivative\ term)$$

$$t ::= q \mid t + t \mid t \& t \mid \qquad (state\ term)$$

$$\vec{t} \mid \pi_X(t) \mid S \mid D$$

Fig. 2: Syntax of terms.

union. Automata terms A specify the set of leaf states of an automaton. Set terms S list a finite number of the leaf states explicitly, while derivative terms D specify them symbolically as states reachable from a set of states S via $\vec{0}$ s. The states themselves are represented by state terms t (notice that set terms S and derivate terms D can both be automata and state terms). Intuitively, the structure of state terms records the automata constructions used to create the top-level automaton from states of the base automata. Non-leaf state terms, the state terms' transition function, and root state terms are then defined inductively from base automata as described below in detail. We will normally use t, u to denote terms of all types (unless the type of the term needs to be emphasized).

Example 1. Consider a formula $\varphi \equiv \neg \exists X. \operatorname{Sing}(X) \land X = \{\epsilon\}$ and its corresponding automata term $t_{\varphi} = \left\{ \overline{\{\pi_X(\{q_0\} \& \{p_0\})\} - \vec{0}^{\frac{1}{N}}\}} \right\}$ (we will show how t_{φ} was obtained from φ later). For the sake of presentation, we will consider the following base automata for the predicates $\operatorname{Sing}(X)$ and $X = \{\epsilon\}$: $\mathcal{A}_{\operatorname{Sing}(X)} = (\{q_0, q_1, q_s\}, \delta, \{q_0\}, \{q_1\})$ and $\mathcal{A}_{X=\{\epsilon\}} = (\{p_0, p_1, p_s\}, \delta', \{p_0\}, \{p_1\})$ where δ and δ' have the following sets of transitions (transitions not defined below go to the sink states q_s and p_s , respectively):

$$\begin{split} \delta: (q_0, q_0) & \neg \{\{X \mapsto 0\}\} \Rightarrow q_0, \ (q_0, q_1) \neg \{\{X \mapsto 0\}\} \Rightarrow q_1, \\ (q_0, q_0) & \neg \{\{X \mapsto 1\}\} \Rightarrow q_1, \ (q_1, q_0) \neg \{\{X \mapsto 0\}\} \Rightarrow q_1 \end{split} \qquad \delta': (p_0, p_0) \neg \{\{X \mapsto 0\}\} \Rightarrow p_0, \\ (p_0, p_0) \neg \{\{X \mapsto 1\}\} \Rightarrow p_1. \end{split}$$

The term t_{φ} denotes the TA $(\pi_X(\mathcal{A}_{\operatorname{Sing}(X)} \cap \mathcal{A}_{X=\{\epsilon\}}) - \vec{0}^{*})^{\mathcal{D}}$ constructed by the operations of intersection, projection, derivative, subset construction, and complement. \square

Semantics of terms. We will define the denotation of an automata term t as the automaton $\mathcal{A}_t = (Q, \Delta, I, R)$. For a set automata term t = S, we define I = S, $Q = reach_{\Delta}(S)$ (i.e., Q is the set of state terms reachable from the leaf state terms), and Δ and R are defined inductively to the structure of t. Particularly, R contains the terms of Q that satisfy the predicate R defined in Fig. 3, and Δ is defined in Fig. 4, with the addition that whenever the rules in Fig. 4 do not apply, then we let $\Delta_a(t,t') = \{\emptyset\}$.

$$\mathcal{R}(t+u) \Leftrightarrow \mathcal{R}(t) \vee \mathcal{R}(u)$$
 (2)

$$\mathcal{R}(t \& u) \Leftrightarrow \mathcal{R}(t) \land \mathcal{R}(u)$$
 (3)

$$\mathcal{R}(\pi_X(t)) \Leftrightarrow \mathcal{R}(t)$$
 (4)

$$\mathcal{R}(\overline{t}) \Leftrightarrow \neg \mathcal{R}(t) \tag{5}$$

$$\mathcal{R}(S) \Leftrightarrow \exists t \in S. \, \mathcal{R}(t)$$
 (6)

$$\mathcal{R}(q) \Leftrightarrow q \in R^{\mathcal{B}}$$
 (7)

Fig. 3: Root term states.

The \emptyset here is used as a universal sink state in order to maintain Δ complete, which is needed for automata terms representing complements to yield the expected language.

The transitions of Δ for terms of the type +, &, π_X , $\overline{\cdot}$, and S are built from the transition function of their sub-terms analogously to how the automata operations of the product union, product intersection, projection, complement, and subset construction, respectively, build the transition function from the transition functions of their arguments (cf. Section 2).

$$\Delta_a(t+u,t'+u') = \Delta_a(t,t') [+] \Delta_a(u,u')$$
 (8)

$$\Delta_a(t \& u, t' \& u') = \Delta_a(t, t') \left[\& \right] \Delta_a(u, u') \tag{9}$$

$$\Delta_a(\pi_X(t), \pi_X(t')) = \{ \pi_X(u) \mid u \in \Delta_{\pi_X(a)}(t, t') \}$$
 (10)

$$\Delta_a(\overline{t}, \overline{t'}) = \{ \overline{u} \mid u \in \Delta_a(t, t') \}$$
 (11)

$$\Delta_a(S, S') = \left\{ \bigcup_{t \in S, t' \in S'} \Delta_a(t, t') \right\}$$
 (12)

$$\Delta_a(q,r) = \delta_a^{\mathcal{B}}(q,r) \tag{13}$$

Fig. 4: Transitions among compatible state terms.

The only difference is that the state terms stay *annotated* with the particular operation by which they were made (the annotation of the set state terms are the set brackets). The root states are also defined analogously as in the classical constructions. In Figs. 3 and 4, the terms t, t', u, u' are arbitrary terms, S, S' are set terms, and $Q, r \in Q^{\mathcal{B}}$.

Finally, we complete the definition of the term semantics by adding the definition of semantics for the derivative term $S - \vec{0}^*$. This term is a symbolic representation of the set term that contains all state terms upward-reachable from S in \mathcal{A}_S over $\vec{0}$. Formally, we first define the so-called *saturation* of \mathcal{A}_S as

$$(S - \vec{0}^{\dagger})^{\mathsf{s}} = reach_{\Delta_{\bar{0}}}(S) \tag{14}$$

(with $reach_{\Delta_{\vec{0}}}(S)$ defined as the fixpoint (1)), and we complete the definition of Δ and \mathcal{R} in Figs. 3 and 4 with three new rules to be used with a derivative term D:

$$\Delta_a(D, u) = \Delta_a(D^{\mathsf{s}}, u) \quad (15) \quad \Delta_a(u, D) = \Delta_a(u, D^{\mathsf{s}}) \quad (16) \qquad \mathcal{R}(D) \Leftrightarrow \mathcal{R}(D^{\mathsf{s}}) \quad (17)$$

The automaton \mathcal{A}_D then equals \mathcal{A}_{D^s} , i.e., the semantics of a derivative term is defined by its saturation.

Example 2. Let us consider a derivative term $t = \{\pi_X(\{q_0\} \& \{p_0\})\} - \vec{0}^*$, which occurs within the nested automata term t_{φ} of Example 1. The set term representing all terms reachable upward from t is then the term

$$t^{s} = \{\pi_{X}(\{q_{0}\} \& \{p_{0}\}), \pi_{X}(\{q_{1}\} \& \{p_{1}\}), \pi_{X}(\{q_{s}\} \& \{p_{s}\}), \pi_{X}(\{q_{1}\} \& \{p_{s}\}), \pi_{X}(\{q_{0}\} \& \{p_{s}\})\}.$$

The semantics of t is therefore the automaton \mathcal{A}_t with the set of states given by t^s . \square

Properties of terms. An implication of the definitions above, essential for termination of our algorithm in Section 4, is that the automata represented by the terms indeed have finitely many states. This is the direct consequence of Lemma 1.

Lemma 1. The size of $reach_{\Delta}(t)$ is finite for any automata term t.

Intuitively, the terms are built over a finite set of states $Q^{\mathcal{B}}$, they are finitely branching, and the transition function on terms does not increase their depth.

Let us further denote by $\mathcal{L}(t)$ the language $\mathcal{L}(\mathcal{A}_t)$ of the automaton induced by a term t. Lemma 2 below shows that languages of terms can be defined from the languages of their sub-terms if the sub-terms are set terms of derivative terms. The terms on the left-hand sides are implicit representations of the automata operations of the respective language operators on the right-hand sides. The main reason why the lemma cannot be extended to all types of sub-terms and yield an inductive definition of term languages is that it is not meaningful to talk about the bottom-up language of an isolated state term that is neither a set term nor a derivative term (which both are also automata terms). This is also one of the main differences from [29] where every term has its own language, which makes the reasoning and the correctness proofs in the current paper significantly more involved.

Lemma 2. For automata terms A_1 , A_2 and a set term S, the following equalities hold:

$$\mathcal{L}(\{A_1\}) = \mathcal{L}(A_1) \tag{a} \qquad \mathcal{L}(\{\overline{A_1}\}) = \overline{\mathcal{L}(A_1)} \tag{d}$$

$$\mathcal{L}(\{A_1 + A_2\}) = \mathcal{L}(A_1) \cup \mathcal{L}(A_2)$$
 (b) $\mathcal{L}(\{\pi_X(A_1)\}) = \pi_X(\mathcal{L}(A_1))$ (e)

$$\mathcal{L}(\{A_1 \& A_2\}) = \mathcal{L}(A_1) \cap \mathcal{L}(A_2)$$
 (c) $\mathcal{L}(S - \vec{0}^*) = \mathcal{L}(S) - \vec{0}^*$

Terms of formulae. Our algorithm in Section 4 will translate a WS2S formula φ into the automata term $t_{\varphi} = \{\langle \varphi \rangle\}$ representing a deterministic automaton with its only leaf state represented by the state term $\langle \varphi \rangle$. The base automata of t_{φ} include the automaton \mathcal{A}_{φ_0} for each atomic predicate φ_0 used in φ . The state term $\langle \varphi \rangle$ is then defined inductively to the structure of φ as shown in Fig. 5. In the defi-

$$\langle \varphi_0 \rangle = I_{\varphi_0} \tag{18}$$

$$\langle \varphi \wedge \psi \rangle = \langle \varphi \rangle \, \& \langle \psi \rangle \tag{19}$$

$$\langle \varphi \lor \psi \rangle = \langle \varphi \rangle + \langle \psi \rangle$$
 (20)

$$\langle \neg \varphi \rangle = \overline{\langle \varphi \rangle} \tag{21}$$

$$\langle \exists X. \ \varphi \rangle = \{ \pi_X(\langle \varphi \rangle) \} - \vec{0}^{\dagger}$$
 (22)

Fig. 5: From formulae to state-terms.

nition, φ_0 is an atomic predicate, I_{φ_0} is the set of leaf states of \mathcal{A}_{φ_0} , and φ and ψ denote arbitrary WS2S formulae. We note that the translation rules may create sub-terms of the form $\{\{t\}\}$, i.e., with nested set brackets. Since $\{\cdot\}$ semantically means determinisation by subset construction, such double determinisation terms can be always simplified to $\{t\}$ (cf. Lemma 2a). See Example 1 for a formula φ and its corresponding term t_{φ} . Theorem 1 establishes the correctness of the formula to term translation.

Theorem 1. Let
$$\varphi$$
 be a WS2S formula. Then $\mathcal{L}(\varphi) = \mathcal{L}(t_{\varphi})$.

The proof of Theorem 1 uses structural induction, which is greatly simplified by Lemma 2, but since Lemma 2 does not (and cannot, as discussed above) cover all used types of terms, the induction step must in some cases still rely on reasoning about the definition of the transition relation on terms.

4 An Efficient Decision Procedure

The development in Section 3 already implies a naïve automata term-based satisfiability check. Namely, by Theorem 1, we know that a formula φ is satisfiable iff $\mathcal{L}(\mathcal{A}_{t_{\varphi}}) \neq \emptyset$.

After translating φ into t_{φ} using rules (18)–(22), we may use the definitions of the transition function and root states of $\mathcal{A}_{t_{\varphi}} = (Q, \Delta, I, F)$ in Section 3 to decide the language emptiness through evaluating the root state test $\mathcal{R}(reach_{\Delta}(I))$. It is enough to implement the equalities and equivalences (8)–(17) as recursive functions. We will further refer to this algorithm as the *simple recursion*. The evaluation of $reach_{\Delta}(I)$ induces nested evaluations of the fixpoint (14): the one on the top level of the language emptiness test and another one for every expansion of a derivative sub-term. The termination of these fixpoint computations is guaranteed due to Lemma 1.

Such a naïve implementation is, however, inefficient and has only disadvantages in comparison to the classical decision procedure. In this section, we will discuss how it can be optimized. Besides an essential *memoization* needed to implement the recursion efficiently, we will show that the automata term representation is amenable to optimizations that cannot be used in the classical construction. These are techniques of state space pruning: the fact that the emptiness can be tested on the fly during the automata construction allows one to avoid exploration of state space irrelevant to the test. The pruning is done through the techniques of *lazy evaluation* and *subsumption*. We will also discuss optimizations of the transition function of Section 3 through *product flattening* and *nondeterministic union*, which are analogies to standard implementations of automata intersection and union.

4.1 Memoization

The simple recursion repeats the fixpoint computations that saturate derivative terms from scratch at every call of the transition function or root test. This is easily countered through *memoization*, known, e.g., from compilers of functional languages, which caches results of function calls in order to avoid their re-evaluation. Namely, after saturating a derivative sub-term $t = S - \vec{0}^{\dagger}$ of t_{φ} for the first time, we simply *replace t* in t_{φ} by the saturation $t^s = reach_{\Delta_{\vec{0}}}(S)$. Since a derivative is a symbolic representation of its saturated version, the replacement does not change the language of t_{φ} . Using memoization, every fixpoint computation is then carried out once only.

4.2 Lazy Evaluation

The *lazy* variant of the procedure uses *short-circuiting* to optimize connectives \land and \lor , and *early termination* to optimize fixpoint computation in derivative saturations. Namely, assume that we have a term $t_1 + t_2$ and that we test whether $\mathcal{R}(t_1 + t_2)$. Suppose that we establish that $\mathcal{R}(t_1)$; we can *short circuit* the evaluation and immediately return true, completely avoiding touching the potentially complex term t_2 (and analogously for a term of the form $t_1 \& t_2$ when one branch is false).

Furthermore, *early termination* is used to optimize fixpoint computations used to saturate derivatives within tests $\mathcal{R}(S-\vec{0}^*)$ (obtained from sub-formulae such as $\exists X.\psi$). Namely, instead of first unfolding the whole fixpoint into a set $\{t_1, \ldots t_n\}$ and only then testing whether $\mathcal{R}(t_i)$ is true for some t_i , the terms t_i can be tested as soon as they are computed, and the fixpoint computation can be stopped early, immediately when the test succeeds on one of them. Then, instead of replacing the derivative sub-term by its full saturation, we replace it by the partial result $\{t_1, \ldots, t_i\} - \vec{0}^*$ for $i \leq n$.

Finishing the evaluation of the fixpoint computation might later be required in order to compute a transition from the derivative. We note that this corresponds to the concept of *continuations* from functional programming, used to represent a paused computation that may be required to continue later.

Example 3. Let us now illustrate the lazy decision procedure on our running example formula $\varphi = \neg \exists X. \operatorname{Sing}(X) \land X = \{\epsilon\}$ and the corresponding automata term $t_{\varphi} = \{\overline{\{\pi_X(\{q_0\} \& \{p_0\})\} - \vec{0}^{\frac{1}{\kappa}}\}}$ from Example 1. The task of the procedure is to compute the value of $\mathcal{R}(\operatorname{reach}_{\Delta}(t_{\varphi}))$, i.e., whether there is a root state reachable from the leaf state $\langle \varphi \rangle$ of $\mathcal{A}_{t_{\varphi}}$. The fact that φ is ground allows us to slightly simplify the problem because any ground formula ψ is satisfiable iff $\bot \in \mathcal{L}(\psi)$, i.e., iff the leaf state $\langle \psi \rangle$ of $\mathcal{A}_{t_{\psi}}$ is also a root. It is thus enough to test $\mathcal{R}(\langle \varphi \rangle)$ where $\langle \varphi \rangle = \{\overline{\pi_X(\{q_0\} \& \{p_0\})\} - \vec{0}^{\frac{1}{\kappa}}}$.

The computation proceeds as follows. First, we use (5) from Fig. 3 to propagate the root test towards the derivative, i.e., to obtain that $\mathcal{R}(\langle \varphi \rangle)$ iff $\neg \mathcal{R}(\{\pi_X(\{q_0\} \& \{p_0\})\} - \vec{0}^{\frac{1}{N}})$. Since the \mathcal{R} -test cannot be directly evaluated on a derivative term, we need to start saturating it into a set term, evaluating \mathcal{R} on the fly, hoping for early termination. We begin with evaluating the \mathcal{R} -test on the initial element $t_0 = \pi_X(\{q_0\} \& \{p_0\})$ of the set. The test propagates through the projection π_X due to (4) and evaluates as false on the left conjunct (through, in order, (3), (6), and (7)) since the state q_0 is not a root state. As a trivial example of short circuiting, we can skip evaluating \mathcal{R} on the right conjunct $\{p_0\}$ and conclude that $\mathcal{R}(t_0)$ is false.

The fixpoint computation then continues with the first iteration, computing the $\vec{0}$ -successors of the set $\{t_0\}$. We will obtain $\Delta_{\vec{0}}(t_0,t_0)=\{t_0,t_1\}$ with $t_1=\pi_X(\{q_1\}\&\{p_1\})$. The test $\mathcal{R}(t_1)$ now returns true because both q_1 and p_1 are root states. With that, the fixpoint computation may terminate early, with the \mathcal{R} -test on the derivative sub-term returning true. Memoization then replaces the derivative sub-term in $\langle \varphi \rangle$ by the partially evaluated version $\{t_0,t_1\}-\vec{0}^{\dagger}$, and $\mathcal{R}(\langle \varphi \rangle)$ is evaluated as false due to (5). We therefore conclude that φ is unsatisfiable (and invalid since it is ground).

4.3 Subsumption

The next technique we use is based on pruning out parts of a search space that are *sub-sumed* by other parts. In particular, we generalize (in a similar way as we did for WS1S in our previous work [29]) the concept used in *antichain* algorithms for efficiently deciding language inclusion and universality of finite word and tree automata [22,23,24,25]. Although the problems are in general computationally infeasible (they are PSPACE-complete for finite word automata and EXPTIME-complete for finite tree automata), antichain algorithms can solve them efficiently in many practical cases.

We apply the technique by keeping set terms in the form of antichains of *simulation-maximal* elements and prune out any other simulation-smaller elements. Intuitively, the notion of a term t being simulation-smaller than t' implies that trees that might be generated from the leaf states $T \cup \{t\}$ can be generated from $T \cup \{t'\}$ too, hence discarding t does not hurt. Formally, we introduce the following rewriting rule:

$$\{t_1, t_2, \dots, t_n\} \rightsquigarrow \{t_2, \dots, t_n\} \qquad \text{for } t_1 \sqsubseteq t_2,$$
 (23)

which may be used to simplify set sub-terms of automata terms. The rule (23) is applied after every iteration of the fixpoint computation on the current partial result. Hence the sequence of partial results is monotone, which, together with the finiteness of $reach_{\Delta}(t)$, guarantees termination. The *subsumption* relation \sqsubseteq used in the rule is defined in Fig. 6 where $S \sqsubseteq^{\forall \exists} S'$ denotes $\forall t \in S \exists t' \in S'$. Intuitively, on base TAs, subsumption

corresponds to inclusion of the set terms (the left disjunct of (24)). This clearly has the intended outcome: a larger set of states can always simulate a smaller set in accepting a tree. The rest of the definition is an inductive extension of the base case. It can be shown that \sqsubseteq for any automata term t is an upward simulation on \mathcal{A}_t in the sense of [25]. Consequently, rewriting sub-terms

$$S \sqsubseteq S' \iff S \subseteq S' \lor S \sqsubseteq^{\forall \exists} S'$$
 (24)

$$t \& u \sqsubseteq t' \& u' \Leftrightarrow t \sqsubseteq t' \land u \sqsubseteq u'$$
 (25)

$$t + u \sqsubseteq t' + u' \Leftrightarrow t \sqsubseteq t' \land u \sqsubseteq u' \tag{26}$$

$$\overline{t} \sqsubseteq \overline{t'} \qquad \Leftrightarrow t' \sqsubseteq t \tag{27}$$

$$\pi_X(t) \sqsubseteq \pi_X(t') \Leftrightarrow t \sqsubseteq t'$$
 (28)

Fig. 6: The subsumption relation \sqsubseteq

in an automata term according to the new rule (23) does not change its language. Moreover, the fixpoint computation interleaved with application of rule (23) terminates.

4.4 Product Flattening

Product flattening is a technique that we use to reduce the size of fixpoint saturations that generate conjunctions and disjunctions of sets as their elements. Consider a term of the form $D = \{\pi_X(S_0 \& S_0')\} - \vec{0}^*$ for a pair of sets of terms S_0 and S_0' where the TAs \mathcal{A}_{S_0} and $\mathcal{A}_{S_0'}$ have sets of states Q and Q', respectively. The saturation generates the set $\{\pi_X(S_0 \& S_0'), \ldots, \pi_X(S_n \& S_n')\}$ with $S_i \subseteq Q, S_i' \subseteq Q'$ for all $0 \le i \le n$. The size of this set is $2^{|Q|\cdot|Q'|}$ in the worst case. In terms of the automata operations, this fixpoint expansion corresponds to first determinizing both \mathcal{A}_{S_0} and $\mathcal{A}_{S_0'}$ and only then using the product construction (cf. Section 2). The automata intersection, however, works for nondeterministic automata too—the determinization is not needed. Implementing this standard product construction on terms would mean transforming the original fixpoint above into the following fixpoint with a flattened product: $D = \{\pi_X(S[\&]S')\} - \vec{0}^*$ where [&] is the augmented product for conjunction. This way, we can decrease the worst-case size of the fixpoint to $|Q| \cdot |Q'|$. A similar reasoning holds for terms of the form $\{\pi_X(S_0 + S_0')\} - \vec{0}^*$. Formally, the technique can be implemented by the following pair of sub-term rewriting rules where S and S' are non-empty sets of terms:

$$S + S' \rightsquigarrow S[+]S',$$
 (29) $S \& S' \rightsquigarrow S[\&]S'.$ (30)

Observe that for terms obtained from WS2S formulae using the translation from Section 3, the rules are not really helpful as is. Consider, for instance, the term $\{\pi_X(\{r\}\&\{q\})\} - \vec{0}^*\}$ obtained from a formula $\exists X.\varphi \land \psi$ with φ and ψ being atoms. The term would be, using rule (30), rewritten into the term $\{\pi_X(\{r\&q\})\} - \vec{0}^*\}$. Then, during a subsequent fixpoint computation, we might obtain a fixpoint of the following form: $\{\pi_X(\{r\&q\}), \pi_X(\{r\&q, r_1\&q_1\}), \pi_X(\{r_1\&q_1, r_2\&q_2\})\}$, where the occurrences of the projection π_X disallow one to perform the desired union of the inner sets, and so the application of rule (30) did not help. We therefore need to equip our procedure with a rewriting rule that can be used to push the projection inside a set term S:

$$\pi_X(S) \leadsto \{\pi_X(t) \mid t \in S\}.$$
 (31)

In the example above, we would now obtain the term $\{\pi_X(r \& q)\} - \vec{0}^*$ (we rewrote $\{\{\cdot\}\}$ to $\{\cdot\}$ as mentioned in Section 3) and the fixpoint $\{\pi_X(r \& q), \pi_X(r_1 \& q_1), \pi_X(r_2 \& q_2)\}$. The correctness of the rules is guaranteed by the following lemma:

Lemma 3. For sets of terms S and S' such that $S \neq \emptyset$ and $S' \neq \emptyset$, we have:

$$\mathcal{L}(\{S+S'\}) = \mathcal{L}(\{S[+]S'\}), \quad (a) \qquad \mathcal{L}(\{\pi_X(S)\}) = \mathcal{L}(\{\pi_X(t) \mid t \in S\}). \quad (c)$$

$$\mathcal{L}(\{S \& S'\}) = \mathcal{L}(\{S[\&]S'\}), \quad (b)$$

However, we still have to note that there is a danger related with the rules (29)–(31). Namely, if they are applied to some terms in a partially evaluated fixpoint but not to all, the form of these terms might get different (cf. $\pi_X(\{r \& q\})$) and $\pi_X(r \& q)$), and it will not be possible to combine them as source states of TA transitions when computing Δ_a , leading thus to an incorrect result. We resolve the situation such that we apply the rules as a pre-processing step only before we start evaluating the top-level fixpoint, which ensures that all terms will subsequently be generated in a compatible form.

4.5 Nondeterministic Union

Optimization of the product term saturations from the previous section can be pushed one step further for terms of the form $\{\pi_X(S+S')\}-\vec{0}^*$. The idea is to use the *nondeterministic TA union* to implement the union operation instead of the product construction. The TA union is implemented as the component-wise union of the two TAs. Its size is hence linear to the size of the input instead of quadratic as in the case of the product (i.e., |Q|+|Q'| instead of $|Q|\cdot|Q'|$). To work correctly, the nondeterministic union requires disjoint input sets of states (otherwise, the combination of the two transition functions could generate runs that are not possible in either of the input TAs). We implement the nondeterministic union through the following rewriting rule:

$$S + S' \leadsto S \cup S' \qquad \text{for } S \not\bowtie S'$$
 (32)

where S and S' are sets of terms (similarly to Section 4.4, in order to successfully reduce the fixpoint state space on terms obtained from WS2S formulae, we also need to apply

rule (31) to push projection inside set terms). The relation \bowtie used in the rule is the *interference* of terms, defined in Fig. 7, which generalizes the state space disjointness requirement of the nondeterministic union of TAs. Interference between terms tells us when we cannot perform the rewriting. Intuitively, this happens when we obtain a term $\{S + S'\}$

$$S \bowtie S' \qquad \Leftrightarrow S = S' \lor \exists t \in S, t' \in S'.t \bowtie t'$$
 (33)

$$t \& u \bowtie t' \& u' \Leftrightarrow t \bowtie t' \lor u \bowtie u' \tag{34}$$

$$t + u \bowtie t' + u' \Leftrightarrow t \bowtie t' \lor u \bowtie u' \tag{35}$$

$$\overline{t} \bowtie \overline{t'} \qquad \Leftrightarrow t \bowtie t'$$
 (36)

$$\pi_X(t) \bowtie \pi_X(t') \Leftrightarrow t \bowtie t'$$
 (37)

$$D\bowtie t \qquad \Leftrightarrow D^{\mathsf{s}}\bowtie t \tag{38}$$

$$t \bowtie D \qquad \Leftrightarrow t \bowtie D^{\mathsf{s}} \tag{39}$$

$$q \bowtie r \qquad \Leftrightarrow \exists 1 \le k \le n. \ q, r \in Q_k$$
 (40)

Fig. 7: Definition of interference ⋈

where S and S' contain states from the same base automaton \mathcal{B}_k with the set of states Q_k .

In order to avoid interference in the terms obtained from WS2S formulae, we can perform the following pre-processing step: When translating a WS2S formula φ into a term t_{φ} , we create a special version of a base TA for every occurrence of an atomic formula in φ . This way, we can never mix up terms that emerged from different subformulae to enable a transition that would otherwise stay disabled.

To use rule (32), it is necessary to modify treatment of the sink state \emptyset in the definition of Δ of Section 3. The technical difficulty we need to circumvent is that (unlike for finite word automata) the nondeterministic union of two (even complete) TAs is not complete.

This can cause situations such as the following: let $D = \{\pi_X(\{\overline{t}\} + \{\overline{r}\})\} - \overline{0}^*$ such that $\Delta_{\overline{0}}(t,t) = \{t\}, \Delta_{\overline{0}}(r,r) = \{r\}$, and $\mathcal{R}(t)$ and $\mathcal{R}(r)$ are both true, i.e., both t and r can accept any $\overline{0}$ -tree, which also means that the union of their complements should not accept any $\overline{0}$ -tree. Indeed, the saturation of D is the set term $D^s = reach_{\overline{0}}(\{\pi_X(\{\overline{t}\} + \{\overline{r}\})\}) = \{\pi_X(\{\overline{t}\} + \{\overline{r}\})\}$ where it holds that $\neg \mathcal{R}(\pi_X(\{\overline{t}\} + \{\overline{r}\}))$, i.e., it does not accept any $\overline{0}$ -tree. On the other hand, if we use the new rule (32) together with rule (31), we obtain the term $\{\pi_X(\overline{t}), \pi_X(\overline{r})\} - \overline{0}^*$. When computing its saturation, we will obtain a new element $\Delta_{\overline{0}}(\pi_X(\overline{t}), \pi_X(\overline{r})) = \pi_X(\overline{0})$. The term $\pi_X(\overline{0})$ was constructed using the implicit rule of Section 3 that sends the otherwise undefined successors of a pair of terms to $\{\emptyset\}$. Note that $\mathcal{R}(\pi_X(\overline{0}))$ is true, yielding that the fixpoint approximation $\{\pi_X(\overline{t}), \pi_X(\overline{r}), \pi_X(\overline{0})\}$ is a root state, so a $\overline{0}$ -tree is accepted. Therefore, the application of the new rule (32) changed the language.

Although the previous situation cannot happen with terms obtained from WS2S formulae using the translation rules from Section 3, in order to formulate a correctness claim for any terms constructed using our grammar, we remedy the issue by modifying the definition of implicit transitions of Δ to $\{\emptyset\}$ from Section 3. Namely, the modified transition function $\Delta_a(t_1,t_2)$ will return the same value as before if $t_1\bowtie t_2$, and otherwise it will return $\{\emptyset\}$. We will denote the modified transition function as Δ' and the corresponding semantics of a term t obtained using Δ' instead of Δ as $\mathcal{L}'(t)$ (Lemmas 2 and 3 and Theorem 1 could be proved similarly with the new definition of semantics). With these new versions of Δ' and \mathcal{L}' , we can show correctness of the rule:

Lemma 4. Let S, S' be sets of terms s.t. $S \not\bowtie S'$. Then $\mathcal{L}'(\{S+S'\}) = \mathcal{L}'(S \cup S')$.

5 Experimental Evaluation

We have implemented the above introduced techniques (so far with the exception of Section 4.5) in a prototype tool written in Haskell.³ The base automata, hard-coded into the tool, were the TAs for the basic predicates from Section 2, together with automata for predicates $\operatorname{Sing}(X)$ and $X = \{p\}$ for a variable X and a fixed tree position p. As an additional optimisation, our tool uses the so-called *antiprenexing* (proposed already in [29]), which pushes quantifiers down the formula tree using the standard logical equivalences. Intuitively, antiprenexing reduces the complexity of elements within fixpoints by removing irrelevant parts outside the fixpoint.

³ The implementation is available at https://github.com/vhavlena/lazy-wsks.

We have performed experiments with our tool on various formulae and compared its performance with that of Mona. We applied Mona both on the original form of the considered formulae as well as on their versions obtained by antiprenexing (which is built into our tool and which—as

Table 1: Experimental results over the family of formulae $\varphi_n^{pt} \equiv \forall Z_1, Z_2. \ \exists X_1, \dots, X_n. \ edge(Z_1, X_1) \land \bigwedge_{i=1}^n edge(X_i, X_{i+1}) \land edge(X_n, Z_2) \ \text{where} \ edge(X, Y) \equiv edge_L(X, Y) \lor edge_R(X, Y) \ \text{and} \ edge_{L/R}(X, Y) \equiv \exists Z. \ Z = S_{L/R}(X) \land Z \subseteq Y.$

	running time (sec)			# of subterms/states		
n	Lazy	Mona	Mona+AP	Lazy	Mona	Mona+AP
1	0.02	0.16	0.15	149	216	216
2	0.50	_	_	937	-	_
3	0.83	_	_	2,487	_	_
4	34.95	_	_	8,391	_	_
5	60.94	_	-	23,827	_	_

we realised—can significantly help Mona too). Our preliminary implementation of product flattening (cf. Section 4.4) is restricted to parts below the lowest fixpoint, and our experiments showed that it does not work well when applied on this level, where the complexity is not too high, so we turned it off for the experiments. We ran all experiments on a 64-bit Linux Debian workstation with the Intel(R) Core(TM) i7-2600 CPU running at 3.40 GHz with 16 GiB of RAM. We used a timeout of 100 s.

We first considered various WS2S formulae on which Mona was successfully applied previously in the literature. On them, our tool is quite slower than Mona, which is not much surprising given the amount of optimisations built into

Table 2: Experimental results over the family of formulae $\varphi_n^{cnst} \equiv \exists X. \ X = \{(\mathtt{LR})^4\} \land X = \{(\mathtt{LR})^n\}.$

	running time (sec)			# of subterms/states		
n	Lazy	Mona	Mona+AP	Lazy	Mona	Mona+AP
80	14.60	40.07	40.05	1,146	27,913	27,913
90	21.03	64.26	64.20	1,286	32,308	32,308
100	28.57	98.42	98.91	1,426	36,258	36,258
110	38.10	_	_	1,566	_	_
120	49.82	_	-	1,706	-	-

Mona (for instance, for the benchmarks from [5], Mona on average took $0.1\,\mathrm{s}$, while we timeouted). Next, we identified several parametric families of formulae (adapted from [29]), such as, e.g., $\varphi_n^{horn} \equiv \exists X. \ \forall X_1. \ \exists X_2, \dots X_n. \ ((X_1 \subseteq X \land X_1 \neq X_2) \Rightarrow X_2 \subseteq X) \land \dots \land ((X_{n-1} \subseteq X \land X_{n-1} \neq X_n) \Rightarrow X_n \subseteq X)$, where our approach finished within $10\,\mathrm{ms}$, while the time of Mona was increasing when increasing the parameter n, going up to $32\,\mathrm{s}$ for n=14 and timeouting for $k\geq 15$. It turned out that Mona could, however, easily handle these formulae after antiprenexing, again (slightly) outperforming our tool. Finally, we also identified several parametric families of formulae that Mona could handle only very badly or not at all, even with antiprenexing, while our tool can handle them much better. These formulae are mentioned in the captions of Tables 1, 2, and 3, which give detailed results of the experiments.

Particularly, Columns 2–4 give the running times (in seconds) of our tool (denoted *Lazy*), Mona, and Mona with antiprenexing. Columns 5–7 characterize the size of the generated terms and automata. Namely, for our approach, we give the number of

Table 3: Experiments over the family $\varphi_n^{sub} = \forall X_1, \dots, X_n$ $\exists X. \ \bigwedge_{i=1}^{n-1} X_i \subseteq X \Rightarrow (X_{i+1} = S_L(X) \lor X_{i+1} = S_R(X)).$

	running time (sec)			# of subterms/states		
n	Lazy	Mona	Mona+AP	Lazy	Mona	Mona+AP
3	0.01	0.00	0.00	140	92	92
4	0.04	34.39	34.47	386	170	170
5	0.24	_	-	981	_	-
6	2.01	_	-	2,376	-	-

nodes in the final term tree (with the leaves being states of the base TAs). For Mona, we give the sum of the numbers of states of all the minimal deterministic TAs constructed by Mona when evaluating the formula. The "—" sign means a timeout or memory shortage.

The formulae considered in Tables 1–3 speak about various paths in trees. We were originally inspired by formulae kindly provided by Josh Berdine, which arose from attempts to translate separation logic formulae to WS2S (and use Mona to discharge them), which are beyond the capabilities of Mona (even with antiprenexing). We were also unable to handle them with our tool, but our experimental results on the tree path formulae indicate (despite the prototypical implementation) that our techniques can help one to handle some complex graph formulae that are out of the capabilities of Mona. Thus, they provide a new line of attack on deciding hard WS2S formulae, complementary to the heuristics used in Mona. Improving the techniques and combining them with the classical approach of Mona is a challenging subject for our future work.

6 Related Work

The seminal works [32,33] on the automata-logic connection were the milestones leading to what we call here the classical tree automata-based decision procedure for WSkS [34]. Its non-elementary worst-case complexity was proved in [35], and the work [2] presents the first implementation, restricted to WS1S, with the ambition to use heuristics to counter the high complexity. The authors of [31] provide an excellent survey of the classical results and literature related to WSkS and tree automata.

The tool Mona [3] implements the classical decision procedures for both WS1S and WS2S. It is still the standard tool of choice for deciding WS1S/WSkS formulae due to its all-around most robust performance. The efficiency of Mona stems from many optimizations, both higher-level (such as automata minimization, the encoding of first-order variables used in models, or the use of multi-terminal BDDs to encode the transition function of the automaton) as well as lower-level (e.g. optimizations of hash tables, etc.) [36,37]. The M2L(Str) logic, a dialect of WS1S, can also be decided by a similar automata-based decision procedure, implemented within, e.g., JMosel [38] or the symbolic finite automata framework of [39]. In particular, JMosel implements several optimizations (such as second-order value numbering [40]) that allow it to outperform Mona on some benchmarks (Mona also provides an M2L(Str) interface on top of the WS1S decision procedure).

The original inspiration for our work are the antichain techniques for checking universality and inclusion of finite automata [22,23,24,25] and language emptiness of alternating automata [41], which use symbolic computation together with subsumption to prune large state spaces arising from subset construction. This paper is a continuation of our work on WS1S, which started by [42], where we discussed a basic idea of generalizing the antichain techniques to a WS1S decision procedure. In [29], we then presented a complete WS1S decision procedure based on these ideas that is capable to rival Mona on already interesting benchmarks. The work in [43] presents a decision procedure that, although phrased differently, is in essence fairly similar to that of [29]. This paper generalizes [29] to WS2S. It is not merely a straightforward generalization of the word concepts to trees. A nontrivial transition was needed from language terms

of [29], with their semantics being defined straightforwardly from the semantics of subterms, to tree automata terms, with the semantics defined as a language of an automaton with transitions defined inductively to the structure of the term. This change makes the reasoning and correctness proof considerably more complex, though the algorithm itself stays technically quite simple.

Finally, Ganzow and Kaiser [44] developed a new decision procedure for the weak monadic second-order logic on inductive structures within their tool Toss. Their approach completely avoids automata; instead, it is based on the Shelah's composition method. The paper reports that the Toss tool could outperform Mona on two families of WS1S formulae, one derived from Presburger arithmetics and one formula of the form that we mention in our experiments as problematic for Mona but solvable easily by Mona with antiprenexing.

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A Proofs

In the proofs we use an alternative definition of automata term semantics. First we bring a notion of a *term expansion* and an *expanded term*. Expanded term does not contain a derivative term as a subterm. Term expansion is then defined recursively as follows: (i) $t^e = t$ if t is expanded. (ii) $t^e = (t[u/u^s])^e$ where u is a derivative term of the form $S - \Gamma^*$ where S is a expanded term. Intuitively in the term expansion, derivative subterms are saturated in a bottom-up manner. Then, we have $\mathcal{L}(\mathcal{A}_{t^e}) = \mathcal{L}(\mathcal{A}_t)$ and therefore, $\mathcal{L}(t^e) = \mathcal{L}(t)$.

Lemma 1. The size of reach $\Delta(t)$ is finite for any automata term t.

Proof. (Sketch) First, we define *depth* of a term t inductively as follows: (i) d(q) = 1 for $q \in Q^{\mathcal{B}}$, (ii) $d(t_1 \circ t_2) = 1 + \max(d(t_1), d(t_2))$ for $oldsymbol{\circ} \in \{\&, +\}$, (iii) $d(\circ t_1) = 1 + d(t_1)$ for $oldsymbol{\circ} \in \{\pi_X, \bar{f}\}$, (iv) $d(S) = 1 + \max_{t \in S}(d(t))$, and (v) $d(S - \Gamma^{\star}) = 1 + d(S)$. Then since the number of reachable states in base automata is finite, for a given n there is a finite number of terms of depth at most n. Moreover, for two terms t_1 and t_2 and each $t \in \Delta_a(t_1, t_2)$ we have $d(t) \leq \max(d(t_1), d(t_2))$. Therefore, for an automaton term S it holds that $\operatorname{reach}_{\Delta}(S)$ is finite.

Lemma 2. For automata terms A_1 , A_2 and a set term S, the following equalities hold:

$$\mathcal{L}(\{A_1\}) = \mathcal{L}(A_1) \tag{a} \qquad \mathcal{L}(\{\overline{A_1}\}) = \overline{\mathcal{L}(A_1)} \tag{d}$$

$$\mathcal{L}(\{A_1 + A_2\}) = \mathcal{L}(A_1) \cup \mathcal{L}(A_2)$$
 (b) $\mathcal{L}(\{\pi_X(A_1)\}) = \pi_X(\mathcal{L}(A_1))$ (e)

$$\mathcal{L}(\lbrace A_1 \& A_2 \rbrace) = \mathcal{L}(A_1) \cap \mathcal{L}(A_2) \quad (c) \qquad \qquad \mathcal{L}(S - \vec{0}^*) = \mathcal{L}(S) - \vec{0}^* \qquad (f)$$

Proof. (a): We prove more general form of (a) namely $\mathcal{L}\left(\{A_1,\ldots,A_n\}\right)=\mathcal{L}\left(\bigcup_{1\leq i\leq n}A_i^{\mathrm{e}}\right)$ (\subseteq) We start with the following reasoning: $\tau\in\mathcal{L}\left(\{A_1,\ldots,A_n\}\right)$ iff there is accepting run ρ on τ in $\mathcal{H}_{\{A_1^{\mathrm{e}},\ldots,A_n^{\mathrm{e}}\}}$ having all leaf states from $\{A_1^{\mathrm{e}},\ldots,A_n^{\mathrm{e}}\}$. For simplicity we set $\Xi=reach_{\Delta}(\bigcup_{1\leq i\leq n}A_i^{\mathrm{e}},\Sigma)$. Moreover, $\forall w\in\mathrm{dom}(\tau)\setminus Leaf(\tau),\ t\in\rho(w)$ we have that $\exists t_1\in\rho(w.\mathrm{L}),t_2\in\rho(w.\mathrm{R}):\ t\in\Delta_{\tau(w)}(t_1,t_2)\subseteq\rho(w)$. Since this run is accepting, there is a $r\in\rho(\epsilon)$ s.t. $\mathcal{R}(r)$. Therefore, we are able to construct the mapping ρ' on $\mathrm{dom}(\tau)$ defined as $\rho'(\epsilon)=r,\rho'(w)\in\Delta_{\tau(w)}(\rho'(w.\mathrm{L}),\rho'(w.\mathrm{R}))$, and $\rho'(w)\in\rho(w)$ for $w\in\mathrm{dom}(\tau)$. Hence $\forall w\in Leaf(\tau):\ \rho'(w)\in\bigcup_{1\leq i\leq n}A_i^{\mathrm{e}}$. It means that $\rho'(w)\in\Xi$ for each $w\in\mathrm{dom}(t)$, and therefore ρ' is an accepting run on τ in $\mathcal{H}_{\bigcup A_i^{\mathrm{e}}}$, i.e., $\tau\in\mathcal{L}\left(\bigcup_{1\leq i\leq n}A_i\right)$.

(\supseteq) Consider $\tau \in \mathcal{L}\left(\bigcup_{1 \leq i \leq n} A_i^{\mathrm{e}}\right)$. Then there is an accepting run ρ on τ in $\mathcal{A}_{\bigcup A_i^{\mathrm{e}}}$. We can then construct the mapping ρ' on $\mathrm{dom}(\tau)$ defined as $\rho'(u) = S_u$ and $\rho'(w) \in \Delta_{\tau(w)}(\rho'(w.\mathtt{L}), \rho'(w.\mathtt{R}))$ for $u \in Leaf(\tau), w \in \mathrm{dom}(\tau)$ where $\rho(u) \in S_u \wedge S_u = A_i$ for some $1 \leq i \leq n$. We have that $\forall w \in \mathrm{dom}(\tau) : \rho(w) \in \rho'(w)$ and therefore ρ' is an accepting run on τ in $\mathcal{A}_{\{A_i^{\mathrm{e}}, \dots, A_n^{\mathrm{e}}\}}$, i.e., $\tau \in \mathcal{L}(\{A_1, \dots, A_n\})$.

(b): (\subseteq) We again start with the reasoning: $\tau \in \mathcal{L}(\{A_1 + A_2\})$ iff there is accepting run ρ on τ in $\mathcal{H}_{\{A_1^e + A_2^e\}}$. Further since ρ is accepting, we can define mappings ρ_1, ρ_2 on

- $\operatorname{dom}(\tau) \text{ s.t. } \forall w \in \operatorname{dom}(\tau): \ \rho_1(w) = l(\rho(w)) \land \rho_1(w) = r(\rho(w)) \text{ where } l(S_1 + S_2) = S_1, \\ r(S_1 + S_2) = S_2. \text{ Moreover, } \rho_1 \text{ is a run on } \tau \text{ in } \mathcal{A}_{\{A_1^e\}} \text{ and } \rho_2 \text{ is a run in } \mathcal{A}_{\{A_2^e\}}. \text{ We also have } \mathcal{R}(\rho(\epsilon)) \text{ hence } \mathcal{R}(\rho_1(\epsilon)) \lor \mathcal{R}(\rho_2(\epsilon)). \text{ Therefore } \tau \in \mathcal{L}\left(\mathcal{A}_{\{A_1^e\}}\right) \lor \tau \in \mathcal{L}\left(\mathcal{A}_{\{A_2^e\}}\right), \\ \text{i.e., } \tau \in \mathcal{L}\left(\{A_1\}\right) \cup \mathcal{L}\left(\{A_2\}\right) \text{ and from } (a) \text{ we get the desired form.}$
- (\supseteq) Consider $\tau \in \mathcal{L}(A_1) \cup \mathcal{L}(A_2)$. From (a) we get $\tau \in \mathcal{L}(\{A_1\}) \cup \mathcal{L}(\{A_2\})$. Then there are runs ρ_1 in $\mathcal{H}_{\{A_1^e\}}$ and ρ_2 in $\mathcal{H}_{\{A_2^e\}}$ on τ s.t. at least one of them is accepting. We can define mapping ρ on $\mathrm{dom}(\tau)$ s.t. $\forall w \in \mathrm{dom}(\tau): \rho(w) = \rho_1(w) + \rho_2(w)$. Such defined mapping is an accepting run on τ in $\mathcal{H}_{\{A_1^e + A_2^e\}}$. Therefore $\tau \in \mathcal{L}(\{A_1 + A_2\})$.
 - (c): Analogy to (b).
- (d): We start with the following reasoning: $\tau \in \mathcal{L}\left(\{\overline{A_1}\}\right)$ iff there is accepting run ρ on τ in $\mathcal{A}_{\{\overline{A_1^e}\}}$. Since in $\mathcal{A}_{\{\overline{A_1^e}\}}$ there is only one leaf state and for each $a \in \Sigma$: $|\Delta_a(\overline{S_1}, \overline{S_2})| \leq 1$, there is at most one accepting run on each tree. The same holds also for $\mathcal{A}_{\{A_1^e\}}$. Note that both $\mathcal{A}_{\{A_1^e\}}$ and $\mathcal{A}_{\{\overline{A_1^e}\}}$ are complete. Therefore ρ is a run on τ in $\mathcal{A}_{\{A_1^e\}}$ iff $\overline{\rho}$ is a run on τ in $\mathcal{A}_{\{A_1^e\}}$ where $\forall w \in \text{dom}(\tau) : \overline{\rho}(w) = \overline{\rho(w)}$. From the definition of \mathcal{R} we further have $\neg \mathcal{R}(\rho(\epsilon)) \Leftrightarrow \mathcal{R}(\overline{\rho}(\epsilon))$. Therefore ρ is not accepting in $\mathcal{A}_{\{A_1^e\}}$ iff $\overline{\rho}$ is accepting in $\mathcal{A}_{\{A_1^e\}}$, which implies $\tau \in L(\mathcal{A}_{\{A_1^e\}})$ iff $\tau \notin L(\mathcal{A}_{\{A_1^e\}})$ and from (a) we get the desired form.
- (e): (\subseteq) Consider $\tau \in \mathcal{L}(\{\pi_X(A_1)\})$. Then there is an accepting run ρ on τ in $\mathcal{A}_{\{\pi_X(A_1^e)\}}$. From the definition of transition function we get that there is the accepting run ρ' on some τ' in $\mathcal{A}_{\{A_1^e\}}$ where $\tau \in \pi_X(\tau')$ and $\forall w \in \text{dom}(\tau) : \rho(w) = \pi_X(\rho'(w))$. Therefore, $\tau \in \pi_X(\mathcal{L}(\{A_1\})) = \pi_X(\mathcal{L}(A_1))$.
- (\supseteq) Consider $\tau \in \pi_X(\mathcal{L}(A_1))$. Then, there is $\tau' \in \mathcal{L}(A_1)$ s.t. $\tau \in \pi_X(\tau')$. According to the part (a), there is an accepting run ρ on τ' in $\mathcal{A}_{\{A_1^e\}}$. Then there is also the accepting run ρ' on τ in $\mathcal{A}_{\{\pi_X(A_1^e)\}}$ where $\forall w \in \text{dom}(\tau): \rho'(w) = \pi_X(\rho(w))$, which concludes the proof.
- (f): We prove more general form of the equality, $\mathcal{L}(A_1) \Gamma^* = \mathcal{L}(A_1 \Gamma^*)$ for a set of symbols Γ . Note that A_1 is a set term. In the following text, for a set term S and a set of symbols Γ we define $S \ominus \Gamma = S^e \cup \bigcup \{\Delta_a(t_1, t_2) \mid t_1, t_2 \in S^e, a \in \Gamma\}$. Note since $\Gamma \subseteq \Sigma$, we have $reach_{\Delta}(S^e, \Sigma) = reach_{\Delta}(S \ominus \Gamma, \Sigma)$. Moreover, a set of trees of height at most n containing symbols from Γ we denote by Γ^n . Formally, $\Gamma^n = \{t \in \Gamma^* \mid \forall w \in \text{dom}(t) : |w| \leq n\}$. Note that |w| denotes the length of a word w. We begin with a claim $\mathcal{L}(S \ominus \Gamma) = \mathcal{L}(S) \Gamma^1$.
- \subseteq : Consider a tree $\tau \in \mathcal{L}(S \ominus \Gamma)$. Therefore there is an accepting run ρ on τ in $\mathcal{A}_{S\ominus\Gamma}$ having leaf states in $S \ominus \Gamma$. Moreover, for each $w \in Leaf(\tau)$ s.t. $\rho(w) \notin S^e$ it holds that $\exists t_{\mathrm{L}}^w, t_{\mathrm{R}}^w \in S^e, a \in \Gamma : \rho(w) \in \Delta_a(t_{\mathrm{L}}^w, t_{\mathrm{R}}^w)$. Hence, we can extend the run ρ to ρ' defined as $\rho'_{|\mathrm{dom}(\tau)} = \rho$ and $\forall w \in Leaf(\tau), \rho(w) \notin S^e : \rho'(w.\mathrm{L}) = t_{\mathrm{L}}^w \wedge \rho'(w.\mathrm{R}) = t_{\mathrm{R}}^w$. The mapping ρ' is a run in \mathcal{A}_{S^e} on a tree $\tau' \in \mathcal{L}(S)$ where $\tau \in \tau' \Gamma^1$, and hence $\tau \in \mathcal{L}(S) \Gamma^1$.
- ⊇: Consider $\tau \in \mathcal{L}(S) \Gamma^1$. Then there is a $\tau' \in \mathcal{L}(S)$ s.t. $\tau \in \tau' \Gamma^1$. Hence there is an accepting run ρ' on τ' in \mathcal{A}_{S^e} . Now consider the set $\Theta = \{w \in Leaf(\tau) \mid \rho'(w) \notin S^e\}$.

Since $\tau \in \tau' - \Gamma^1$, we have $\forall w \in \Theta : \rho'(w.L) \in S^e \land \rho'(w.R) \in S^e \land \tau'(w) \in \Gamma$. Therefore, $\rho = \rho'_{|\text{dom}(\tau)}$ is an accepting run on τ in $\mathcal{A}_{S \ominus \Gamma}$, i.e., $\tau \in \mathcal{L}(S \ominus \Gamma)$.

We proceed to main part of the lemma. Consider a sequence of automata terms $S_0 = S^{\rm e}$, $S_1 = S_0 \ominus \Gamma$, $S_{i+1} = S_i \ominus \Gamma$. Because the set of all terms that can occur in S_i is finite (Lemma 1), there is some n_0 s.t. for all $n'' \ge n_0$ and $n' \ge n_0$ we have $S_{n'} = S_{n''}$. Moreover, $S_{n_0} = reach_{\Delta}(S^{\rm e}, \Gamma)$. From the previous claim we have $\mathcal{L}(S_i) = \mathcal{L}(S) - \Gamma^i$ and consequently $\bigcup_{i \ge 1} \mathcal{L}(S_i) = \bigcup_{i \ge 1} \mathcal{L}(S) - \Gamma^i = \mathcal{L}(S) - \Gamma^*$. Moreover from the previous reasoning we have $\mathcal{L}(S_{n'}) = \mathcal{L}(S_{n''})$ for $n'' \ge n_0$, $n' \ge n_0$. Hence $\bigcup_{i \ge 1} \mathcal{L}(S_i) = \mathcal{L}(S_{n_0})$ (follows from $\mathcal{L}(S_i) \subseteq \mathcal{L}(S_{i+1})$). Finally we have $\mathcal{L}(S_{n_0}) = \mathcal{L}(reach_{\Delta}(S^{\rm e}, \Gamma)) = \mathcal{L}(S - \Gamma^*) = \mathcal{L}(S) - \Gamma^*$.

Theorem 1. Let φ be a WS2S formula. Then $\mathcal{L}(\varphi) = \mathcal{L}(t_{\varphi})$.

Proof. For the purpose of this proof we restrict the definition of terms to *deterministic terms* constructed using the following grammar:

$$D ::= \{d, \dots, d\} \mid \{\pi_X(d), \dots, \pi_X(d)\}$$
 (41)

$$d ::= S \mid d + d \mid d \& d \mid \overline{d} \mid D \mid D - \Gamma^{*}$$
 (42)

where D is a finite set of deterministic terms and S is a finite set of terms. Note that for two expanded deterministic terms t_1 , t_2 we have $|\Delta_a(t_1, t_2)| = 1$. Further note that for a WS2S formula φ , $\langle \varphi \rangle$ is a deterministic term.

Now, we prove $\mathcal{L}(\varphi) = \mathcal{L}(\{\langle \varphi \rangle\})$ by a structural induction on φ . We use properties of the classical decision procedure.

- $-\varphi = \varphi_0$ where φ_0 is an atomic formula: From the translation formula to terms and Lemma 2 (a) we directly have $\mathcal{L}(\varphi_0) = \mathcal{L}(\langle \varphi_0 \rangle) = \mathcal{L}(\langle \varphi_0 \rangle)$.
- $-\varphi = \psi_1 \wedge \psi_2$: From the translation formula to terms and Lemma 2 (a) we get

$$\mathcal{L}(\{\langle \varphi \rangle\}) = \mathcal{L}(\{\langle \psi_1 \rangle \& \langle \psi_2 \rangle\}) = \mathcal{L}(\{\{\langle \psi_1 \rangle \& \langle \psi_2 \rangle\}\}). \tag{43}$$

Further, from (43), Lemma 3 and Lemma 2 (c) we obtain

$$\mathcal{L}(\{\{\langle \psi_1 \rangle \& \langle \psi_2 \rangle\}\}) = \mathcal{L}(\{\{\langle \psi_1 \rangle\} \& \{\langle \psi_2 \rangle\}\}) = \mathcal{L}(\{\langle \psi_1 \rangle\}) \cap \mathcal{L}(\{\langle \psi_2 \rangle\}). \tag{44}$$

Finally from IH we have $\mathcal{L}(\{\langle \varphi \rangle\}) = \mathcal{L}(\psi_1) \cap \mathcal{L}(\psi_2) = \mathcal{L}(\varphi)$.

 $-\varphi = \psi_1 \vee \psi_2$: From the translation formula to terms and Lemma 2 (a) we get

$$\mathcal{L}(\{\langle \varphi \rangle\}) = \mathcal{L}(\{\langle \psi_1 \rangle + \langle \psi_2 \rangle\}) = \mathcal{L}(\{\{\langle \psi_1 \rangle + \langle \psi_2 \rangle\}\}). \tag{45}$$

Further, from (45), Lemma 3 and Lemma 2 (b) we obtain

$$\mathcal{L}(\{\{\langle \psi_1 \rangle\} + \{\langle \psi_2 \rangle\}\}) = \mathcal{L}(\{\langle \psi_1 \rangle\}) \cup \mathcal{L}(\{\langle \psi_2 \rangle\}). \tag{46}$$

Finally from IH we have $\mathcal{L}(\{\langle \varphi \rangle\}) = \mathcal{L}(\psi_1) \cup \mathcal{L}(\psi_2) = \mathcal{L}(\varphi)$.

 $-\varphi = \neg \psi$: First, we prove the following claim: Let t be a deterministic term, then $\mathcal{L}\left(\left\{\overline{\{t\}}\right\}\right) = \mathcal{L}\left(\left\{\overline{t}\right\}\right)$. Proof: First consider two expanded deterministic terms t_1, t_2 . Since t_1, t_2 are deterministic, we have $\Delta_a(\underline{t_1}, \underline{t_2}) = \{t'\}$ for some deterministic term t'. Therefore, $\Delta_a(\overline{t_1}, \overline{t_2}) = \{\overline{t'}\}$ and $\Delta_a(\{t_1\}, \{t_2\}) = \{\overline{t'}\}$. Hence, there is an accepting run ρ on a tree τ in $\mathcal{A}_{\left\{\overline{t}\right\}}$ iff there is an accepting run ρ' on a tree τ in

 $\mathcal{A}_{\{\overline{t}\}} \text{ where } \forall w \in \mathrm{dom}(\tau): \ \rho(w) = \overline{s} \wedge \rho'(w) = \overline{\{s\}}.$

We proceed in the main part of the theorem. From the translation formula to terms and from the previous claim we get

$$\mathcal{L}\left(\left\{\left\langle \varphi\right\rangle\right\}\right) = \mathcal{L}\left(\left\{\overline{\left\langle \psi\right\rangle}\right\}\right) = \mathcal{L}\left(\left\{\overline{\left\{\left\langle \psi\right\rangle\right\}}\right\}\right). \tag{47}$$

Finally from (47), Lemma 2 (d) and IH we have

$$\mathcal{L}\left(\left\{\left\langle \varphi\right\rangle\right\}\right) = \overline{\mathcal{L}\left(\left\{\left\langle \psi\right\rangle\right\}\right)} = \overline{\mathcal{L}\left(\psi\right)} = \mathcal{L}\left(\varphi\right). \tag{48}$$

 $-\varphi=\exists X.\ \psi$: First, we prove the following claim: Let t be a deterministic term, then $\mathcal{L}\left(\{\pi_X(\{t\})\}\right)=\mathcal{L}\left(\{\pi_X(t)\}\right)$. Proof: First consider two expanded deterministic terms t_1,t_2 . Since t_1,t_2 are deterministic, for each a we have $\Delta_a(t_1,t_2)=\{t_a\}$ for some deterministic term t_a . Therefore, $\Delta_a(\pi_X(t_1),\pi_X(t_2))=\{\pi_X(t_b)\ |\ b\in\pi_X(a)\}$ and $\Delta_a(\pi_X(\{t_1\}),\pi_X(\{t_2\}))=\{\pi_X(\{t_b\})\ |\ b\in\pi_X(a)\}$. Hence, there is an accepting run ρ on a tree τ in $\mathcal{R}_{\{\pi_X(t)\}}$ where $\forall w\in \mathrm{dom}(\tau):\ \rho(w)=\pi_X(s)\land\rho'(w)=\pi_X(\{s\})$.

We proceed in the main part of the theorem. From the translation formula to terms we get

$$\mathcal{L}\left(\left\{\left\langle \varphi\right\rangle\right\}\right) = \mathcal{L}\left(\left\{\pi_X(\left\langle \psi\right\rangle\right\}\right\} - \vec{0}^*\right) \tag{49}$$

Further, from (49), Lemma 2 (f), and the previous claim we have

$$\mathcal{L}(\{\langle \varphi \rangle\}) = \mathcal{L}(\{\pi_X(\langle \psi \rangle)\}) - \vec{0}^{\dagger} = \mathcal{L}(\{\pi_X(\{\langle \psi \rangle\})\}) - \vec{0}^{\dagger}. \tag{50}$$

Then from (50) and Lemma 2 (e) we obtain

$$\mathcal{L}(\{\langle \varphi \rangle\}) = \pi_X \left(\mathcal{L}(\{\langle \psi \rangle\}) \right) - \vec{0}^{\dagger}. \tag{51}$$

IH together with (51) give us

$$\mathcal{L}(\{\langle \varphi \rangle\}) = \pi_X(\mathcal{L}(\psi)) - \vec{0}^{\dagger} = \mathcal{L}(\varphi). \tag{52}$$

Finally, we have $L(\varphi) = \mathcal{L}(\{\langle \varphi \rangle\})$.

Lemma 3. For sets of terms S and S' such that $S \neq \emptyset$ and $S' \neq \emptyset$, we have:

$$\mathcal{L}(\{S+S'\}) = \mathcal{L}(\{S[+]S'\}), \quad (a) \qquad \mathcal{L}(\{\pi_X(S)\}) = \mathcal{L}(\{\pi_X(t) \mid t \in S\}). \quad (c)$$

$$\mathcal{L}(\{S \& S'\}) = \mathcal{L}(\{S[\&]S'\}), \quad (b)$$

Proof. (a): (\subseteq): Consider some $\tau \in \mathcal{L}(\{S+S'\})$. From Lemma 2 we have $\mathcal{L}(\{S+S'\}) = \mathcal{L}(S) \cup \mathcal{L}(S')$. Hence there are runs ρ_1 in \mathcal{A}_{S^e} and ρ_2 in $\mathcal{A}_{S'^e}$ on τ and at least one them is accepting (both runs exist since the transition function Δ is total). Then, we can construct a mapping ρ on dom(τ) defined as $\forall w \in \text{dom}(\tau) : \rho(w) = \rho_1(w) + \rho_2(w)$. The ρ is a run on τ in $\mathcal{A}_{\{t_1^e+t_2^e \mid t_1 \in S, t_2 \in S'\}}$. Moreover, this run is accepting since ρ_1 or ρ_2 is accepting. Therefore, $\tau \in \mathcal{L}(\{t_1 + t_2 \mid t_1 \in S, t_2 \in S'\})$ and from Lemma 2 $\tau \in \mathcal{L}(\{S \mid \& \} S'\})$.

(\supseteq): Consider some $\tau \in \mathcal{L}(\{S \ [\&] \ S'\})$. Then from Lemma 2 we obtain that $\tau \in \mathcal{L}(\{t_1+t_2 \mid t_1 \in S, t_2 \in S'\})$. Then, there is the accepting run ρ on τ in $\mathcal{A}_{\{t_1^e+t_2^e \mid t_1 \in S, t_2 \in S'\}}$. Further, we are able to construct the run ρ' on $\mathrm{dom}(\tau)$ in $\mathcal{A}_{\{S+S'\}}$ such that $\forall w \in \mathrm{dom}(\tau): \rho'(w) = S_1 + S_2$ where $\rho(w) = t_1 + t_2, t_1 \in S_1 \wedge t_2 \in S_2$. Since ρ is accepting, ρ' is accepting as well. Therefore, $\tau \in \mathcal{L}(\{S+S'\})$.

(b): Analogy to (a).

(c): From Lemma 2 we have that $\mathcal{L}(\{\pi_X(S)\}) = \pi_X(\mathcal{L}(S))$. We prove that $\pi_X(\mathcal{L}(S)) = \mathcal{L}(\{\pi_X(t) \mid t \in S\})$.

(\subseteq): Consider some $\tau \in \pi_X(\mathcal{L}(S))$. Then, there is a tree $\tau' \in \mathcal{L}(S)$ such that $\tau \in \pi_X(\tau')$. Therefore, there is a accepting run ρ on τ' in \mathcal{A}_{S^e} and hence there is the accepting run ρ' on τ' in $\mathcal{A}_{\{\pi_X(t) \mid t \in S^e\}}$ defined as $\forall w \in \text{dom}(\tau) : \rho'(w) = \pi_X(\rho(w))$ which implies $\tau \in \mathcal{L}(\{\pi_X(t) \mid t \in S\})$.

(\supseteq): Consider $\tau \in \in \mathcal{L}(\{\pi_X(t) \mid t \in S\})$. Therefore, threre is an accepting run ρ' on some τ' in \mathcal{A}_{S^e} defined as $\forall w \in \text{dom}(\tau) : \rho'(w) = t$ where $\rho(w) = \pi_X(t)$. Moreover, we have $\tau \in \pi_X(\tau')$. Hence $\tau \in \pi_X(\mathcal{L}(S))$.

Lemma 4. Let S, S' be sets of terms s.t. $S \not\bowtie S'$. Then $\mathcal{L}'(\{S+S'\}) = \mathcal{L}'(S \cup S')$.

Proof. (\subseteq): From Lemma 2 for a modified transition function, we have $\mathcal{L}'(\{S+S'\}) = \mathcal{L}'(S) \cup \mathcal{L}'(S')$. Now assume $\tau \in \mathcal{L}'(S) \cup \mathcal{L}'(S')$. Then, there is an accepting run ρ on τ either in \mathcal{A}_{S^e} or in $\mathcal{A}_{S'^e}$. Therefore, ρ is an accepting run on τ also in $\mathcal{A}_{S^e \cup S'^e}$.

(\supseteq): We assume that $\tau \in \mathcal{L}'(S \cup S')$. Since for each $t_1 \in S^e$ and $t_2 \in S'^e$ holds $t_1 \not\bowtie t_2$, we have that $t \in \Delta'_a(t_1, t_2)$ is equal to \emptyset (and vice versa). Therefore, if ρ is an accepting run on τ in $\mathcal{A}_{S^e \cup S'^e}$, then ρ is an accepting run in \mathcal{A}_{S^e} or in $\mathcal{A}_{S'^e}$. Hence, $\tau \in \mathcal{L}'(\{S + S'\})$.

B Basic WSkS Predicates

$$X = \emptyset \Leftrightarrow \forall Y. \ X \subseteq Y \tag{53}$$

$$\operatorname{Sing}(X) \Leftrightarrow \forall Y. Y \subseteq X \Rightarrow Y = X \land Y = \emptyset$$
 (54)

C Basic TAs

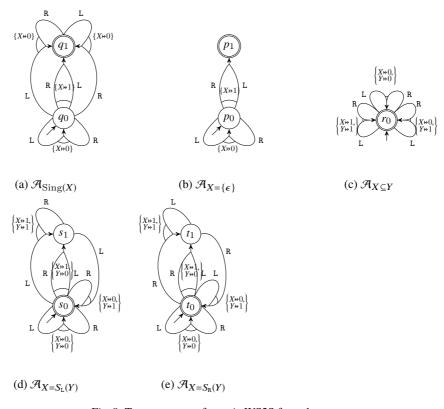


Fig. 8: Tree automata of atomic WS2S formulae.