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Deciding Twig-definability of Node Selecting Tree Automata

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Abstract Node selecting tree automata (NSTAs) constitute a general formalism defining unary queries over trees. Basically, a node is selected by an NSTA when it is visited in a selecting state during an accepting run. We consider twig patterns as an abstraction of XPath. Since the queries definable by NSTAs form a strict superset of twig-definable queries, we study the complexity of the problem to decide whether the query by a given NSTA is twig-definable. In particular, we obtain that the latter problem is EXPTIME-complete. In addition, we show that it is also EXPTIME-complete to decide whether the query by a given NSTA is definable by a node selecting string automaton.

Keywords Automata · Twigs · Complexity · Definability

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1 Introduction

As node selecting queries are fundamental in the context of tree-structured data like XML and web documents, many formalisms expressing such unary queries over trees have been investigated over time. Surprisingly many formalisms have been proposed which are expressively equivalent to the unary queries definable in monadic second-order logic (MSO) turning the latter into a yardstick for expressiveness over tree-structured data. We refer to these queries as the *regular unary queries*. Expressively equivalent formalisms are for instance based on attribute grammars [28,29], automata [13,16,31], and logic [12,19,30]. Though expressive, well-understood, and robust, regular unary queries lack the simplicity and usability of less expressive languages like for instance XPath. Furthermore, a major advantage of XPath is without doubt the large body of research on efficient evaluation, optimization, and static analysis (see, e.g. [5] for a survey) and the availability of implementations. As such results for general unary regular queries are scarce, the goal of the present paper is to investigate the problem to decide whether a given regular unary query can in fact already be defined in an XPath-like formalism.

The proposed type of research has attracted a lot of attention in the area of logic and automata. There, a logic is said to have a decidable characterization if the following decision problem is decidable: "Given as input a finite automaton, decide if the recognized language can be defined using a formula of the logic". Although quite a bit of research is available for logics over trees (cf., e.g., [6,10,37]), the most directly related result is by Place and Segoufin who showed that it is decidable whether a regular unranked tree language is definable in FO_2 over the descendant and the following-sibling axes [33]. In terms of expressive power the latter logic corresponds to a fragment of the navigational core of XPath that contains modalities for going up to some ancestor, down to some descendant, left to some preceding sibling, and right to some following sibling. The devised decision problem leads to a high complexity with several nested exponentials. Although it is open whether this high complexity is unavoidable, in this paper, we do not consider FO_2 over trees but restrict our attention to some of its fragments. Another related result is the one by Bojańczyk and Walukiewicz [11] showing that Boolean definability in the logic EX+EF is decidable in EXPTIME w.r.t. a given nondeterministic binary tree automaton. In short, the logic EX+EF is defined over binary trees, expresses the child and ancestor relation and is closed under the Boolean connectives. Specifically, we consider regular path queries and XPath with child, descendant and filter.[1] We refer to the latter as twig queries. These twig queries are incomparable to EX+EF as they are defined over unranked trees and can define unary queries but are not closed under Boolean operations. To represent unary regular queries, we employ the class of node selecting tree automata (NSTA) as defined in [16,26] extended with wildcards. Basically, an NSTA is a nondeterministic unranked tree automaton with a distinguished set of *selecting* states. A node is then selected by an NSTA when it is visited in a selecting state during an accepting run. The output of the automaton consists of all selected nodes.

[1] *Filter* is sometimes also called *predicate*, e.g., in the XPath specification by the World Wide Web Consortium.

A regular path query selects a node based on regular properties of its ancestor-string, that is, the string formed by the labels on the path from the root to that node. We formalize the latter as NFA-definable queries. Specifically, an NFA can express a unary query by selecting every node which is visited in an accepting state on the path from the root to that node. We characterize the NFA-definable regular queries as those regular queries which are ancestor-based. The latter is a formalization of the idea that NFA-definable queries cannot distinguish between nodes with the same ancestor-string. Using this insight, we construct an NFA $\mathsf{NFA}(M)$ for a given NSTA M, such that M is equivalent to $\mathsf{NFA}(M)$ if and only if the query defined by M is NFA-definable. We then show that the latter equivalence test can be performed in exponential time. Altogether, we show that testing NFA-definability of NSTAs is EXPTIME-complete. We further discuss the relationship with ancestor-based types for XML schema languages as defined in [23] and address tractability.

Next, we turn to twig queries which are tree-patterns consisting of child and descendant edges. These correspond to the fragment of XPath restricted to child-axis, descendant-axis and filter. We show that NSTAs can be exponentially more succinct than twig queries. However, the large size of such twigs is due to a high degree of duplication which can be significantly reduced by folding them. We refer to the latter as DAG-twigs where DAG stands for a directed acyclic graph. In particular, we show that when an NSTA is twig-definable, there always exists an equivalent DAG-twig of at most linear size. To test twig-definability of NSTAs, one can simply guess a DAG-twig of linear size and test equivalence with the given NSTA. We show that the latter equivalence test can be done in EXPTIME through a reduction to emptiness of alternating tree-walking automata. The main result of this paper is that testing twig-definability of NSTAs is complete for EXPTIME.

Related Work. Various properties of XPath have been investigated in the literature as for instance, its complexity, containment, and expressiveness. The complexity of XPath and efficient evaluation algorithms are investigated in, e.g., [20,21,9]. The containment and satisfiability problems for XPath have been deeply studied in the database literature, for example in [25,32,8,36]. The expressiveness of various fragments and extensions of XPath have been investigated in, e.g., [4,24,37]. We refer to [5,34] for surveys on these problems. To the best of our knowledge the above mentioned results of Place and Segoufin [33] and Bojańczyk and Walukiewicz [11] are the only research which studies decidability of XPath definability.

Outline. In Section 2, we introduce the necessary definitions. In Section 3, we discuss regular path-definability of NSTAs. In Section 4, we discuss twig-definability of NSTAs. We conclude in Section 5.

2 Definitions

Here, we introduce the necessary definitions concerning trees, queries and automata. For a finite set S, we denote by $|S|$ its number of elements.

2.1 Trees

Let Δ always denote an infinite set of *labels*. Intuitively, Δ is our abstraction of the set of XML-tags. We assume that we can test equality between elements from Δ in constant time. We denote by Δ^* the set of finite strings over Δ. By ε we denote the empty string. We only consider rooted, ordered, finite, labelled, unranked trees which are directed from the root downwards. That is, we consider trees with a finite number of nodes and in which nodes can have arbitrarily many children. We view a tree t as a relational structure over a finite number of unary labelling relations $\sigma(\cdot)$, where each $\sigma \in \Delta$, and binary relations child$(\cdot,\cdot)$ and next-sibling$(\cdot,\cdot)$. Here, $\sigma(u)$ expresses that u is a node with label σ, and child(u,v) (respectively, next-sibling(u,v)) expresses that v is a child (respectively, the next sibling) of u. When next-sibling(u,v) holds, we sometimes also say that v is (immediately) to the right of u. We write Nodes^t for the set of nodes of t. The set of edges of a tree t, denoted by Edges^t is the set of pairs (u,v) such that child(u,v) holds in t. The root node of t is denoted by $\mathsf{root}(t)$. We define the *size of* t, denoted by $|t|$, to be the number of nodes of t. By $\sigma(t_1,\ldots,t_n)$ we denote a tree with root labelled σ and subtrees $t_1,\ldots,t_n$ attached below the root from left to right. We sometimes overload notation and denote by σ not only the Δ-symbol but also the tree that has a σ-labelled root and no children below the root. By $\mathscr{T}_\Delta$ we denote the set of all trees.

A *path* in tree t is a sequence of nodes $v_0 \cdots v_n$ such that, for each $i = 1,\ldots,n$, we have that $(v_{i-1},v_i) \in \mathsf{Edges}^t$. Paths therefore never run upwards, that is, turn towards to the root of t. We say that $v_0 \cdots v_n$ is a path *from* v_0 *to* v_n and that the *length* of the path is n. The *depth* of a node $v \in \mathsf{Nodes}^t$ is equal to the length of the (unique) path from $\mathsf{root}(t)$ to v. The *height* of a tree t is then defined as the maximum of the depths of all its nodes.

The label of each node v in t must be defined and unique, that is, for each node $v \in \mathsf{Nodes}^t$ there exists a unique $\sigma \in \Delta$ such that $\sigma(v)$ holds. We denote the label of v in t by $\mathsf{lab}^t(v)$. For a node v in a tree t, the *ancestor-string* of v, denoted $\mathsf{ancstr}^t(v)$, is the concatenation of the labels on all the nodes on the path from the root to v, including the two latter nodes. More specifically, $\mathsf{ancstr}^t(v)$ is the sequence $\mathsf{lab}^t(v_0)\cdots\mathsf{lab}^t(v_n)$, where $v_0 \cdots v_n$ is the path from $\mathsf{root}(t)$ to v. For a tree t and a node $v \in \mathsf{Nodes}^t$, the *subtree of* t *at* v, denoted by $\mathsf{subtree}^t(v)$, is the tree induced by all the nodes u such that there is a (possibly empty) path from v to u. In particular, for any tree t and leaf node v, $\mathsf{subtree}^t(v) = \mathsf{lab}^t(v)$ and, for any other node u, $\mathsf{subtree}^t(u) = \mathsf{lab}^t(u)(\mathsf{subtree}^t(u_1),\ldots,\mathsf{subtree}^t(u_n))$, where $u_1,\ldots u_n$ are the children of u from left to right.

Similarly, the *context of* t *at* v, denoted by $\mathsf{context}^t(v)$, is the tree induced by v and all the nodes that are *not* reachable by a path from v and which has a special marker at the position of v. In particular, $\mathsf{context}^t(v)$ is defined inductively as follows. Let $\mathsf{context}^t(\mathsf{root}(t)) = \#$ for some $\# \notin \Delta$. If v is not the root of t, let u be the parent of v and let the children of u be $v_1,\ldots,v_n$, from left to right. Assume that $v = v_i$. Then, $\mathsf{context}^t(v)$ is the tree obtained by replacing the unique #-labelled node in $\mathsf{context}^t(u)$ with the tree

$$\mathsf{lab}^t(u)\big(\mathsf{subtree}^t(v_1),\ldots,\mathsf{subtree}^t(v_{(i-1)}),\#,\mathsf{subtree}^t(v_{(i+1)}),\ldots,\mathsf{subtree}^t(v_n)\big)$$

By $t[v \leftarrow t']$ we denote the tree constructed from t by replacing $\mathsf{subtree}^t(v)$ at node v with t'. In other words, assuming w.l.o.g. that the sets of nodes in t and t' are disjoint, $t[v \leftarrow t']$ is the tree obtained by replacing the #-labelled node in $\mathsf{context}^t(v)$ with the tree t'.

2.2 Expressions and Automata

Throughout the paper, $\Sigma \subseteq \Delta$ always denotes a finite alphabet. The set of *regular expressions* with symbols from a finite alphabet Σ is denoted by $\mathscr{R}_\Sigma$. We use standard regular expressions using the operators $\cdot$ (concatenation), $+$ (disjunction), and * (Kleene star). For a regular expression r, $L(r)$ is the language of the expression, and $\mathsf{Labels}(r)$ is the set of labels occurring in r. The *size* of a regular expression r, denoted by $|r|$, is defined as the length of its string representation.

The twig pattern queries we consider in this paper (see Section 4 for a formal definition) use only a finite set of labels, but the trees that match it can use arbitrary labels from an infinite set. This is to conform with the XPath query language, on which twig pattern queries are inspired. However, automata usually only use a finite alphabet of labels. To overcome this discrepancy we will use a wildcard symbol "$\diamond$" that will give automata the same power. We assume that the single-symbol wildcard symbol $\diamond$ is not in Δ and we denote $\Sigma \uplus \{\diamond\}$ by $\Sigma_\diamond$.

We define non-deterministic finite automata (NFAs) and their languages in the usual way, with the additional feature of a wildcard symbol that can match any Δ-symbol not in Σ. An *NFA$_w$(NFA with wildcards)* is a tuple $A = (\Sigma, Q, q_I, \delta, F)$, where Q is the finite set of states, $q_I \in Q$ is the initial state, $F \subseteq Q$ is the set of final states, and $\delta : Q \times \Sigma_\diamond \to 2^Q$ is the transition function. From the transition function δ, we define the extended transition function $\delta^* : (Q \times \Delta^*) \to 2^Q$ which can read entire Δ-strings. In particular, $\delta^*(q, \varepsilon) = \{q\}$, $\delta^*(q,a) = \delta(q,a)$ if $a \in \Sigma$, $\delta^*(q,a) = \delta(q,\diamond)$ if $a \in \Delta - \Sigma$, and $\delta^*(q, a \cdot w) = \cup_{q' \in \delta^*(q,a)} \delta^*(q', w)$, where $a \in \Delta$ and $w \in \Delta^*$. A word $w \in \Delta^*$ is accepted by A if $\delta^*(q_I, w) \cap F \neq \emptyset$. The set of words accepted by A is denoted by $L(A)$. The *size* of A, denoted by $|A|$, is defined as $|Q| + \sum_{q \in Q, a \in \Sigma_\diamond} |\delta(q,a)|$.

A *nondeterministic tree automaton with wildcards* or *NTA$_w$* is a tuple $N = (\Sigma, Q, \delta, F)$ where Q is a finite set of states, $F \subseteq Q$ is the set of final states, and the transition function $\delta : Q \times \Sigma_\diamond \to \mathscr{R}_Q$ is a mapping from pairs of a state and a label to regular expressions over Q. Again, transitions labelled by $\diamond$ can be followed by reading any symbol not in Σ.

A *run* of N on a tree t is an assignment of states to nodes $\lambda : \mathsf{Nodes}^t \to Q$ such that, for every $v \in \mathsf{Nodes}^t$ with n children $v_1, \ldots, v_n$ from left to right, the following holds: if $\mathsf{lab}^t(v) \in \Sigma$, then

$$\lambda(v_1) \cdots \lambda(v_n) \in L(\delta(\lambda(v), \mathsf{lab}^t(v))). \tag{2.1}$$

and if $\mathsf{lab}^t(v) \in \Delta - \Sigma$, then

$$\lambda(v_1) \cdots \lambda(v_n) \in L(\delta(\lambda(v), \diamond)). \tag{2.2}$$

When v has no children, the criterion reduces to

$$\varepsilon \in L(\delta(\lambda(v), \mathsf{lab}^t(v))) \quad \text{or} \quad \varepsilon \in L(\delta(\lambda(v), \diamond)).$$

A run is *accepting* if the root is labelled with a state in F. A tree t is *accepted* by N if there is an accepting run of N on t. The set of all trees accepted by N is denoted by $L(N)$. If $L(N) = \mathscr{T}_\Delta$, we call N *universal*. The *size* of N is defined as $|Q| + \sum_{q\in Q, a\in\Sigma_\diamond} |\delta(q,a)|$. We say that two NTA$_w$s are *equivalent* if they define the same language.

For any $p \in Q$, let $N_p = (\Sigma, Q, \delta, \{p\})$. We call p *universal in* N if N_p is universal. We say that a state p is *reachable* from a state q, if $p = q$, or if there is an $a \in \Delta$ and $w_1 q' w_2 \in L(\delta(q,a))$ such that p is reachable from q'.

Notice that, in our automata definitions, we could have let a wildcard match any Δ-symbol rather than any symbol in $\Delta - \Sigma$. While at first sight it may seem more natural to some to let the wildcard match any Δ-symbol, we note that the variant we chose here is more powerful. Indeed, the former semantics can be simulated by the latter (by simply adding an extra transition for every Σ-symbol) but not vice versa. For example, the latter variant can test if a label is in $\{a\} \cup (\Delta - \Sigma)$ with $a \in \Sigma$, whereas the former cannot. We therefore chose the more powerful variant.

Unless explicitly mentioned otherwise, we will assume that NTA$_w$s do not have *useless* states. That is, for each state q, there is at least one accepting run λ of the NTA$_w$ on some tree t where $\lambda(u) = q$ for some node u of t. We justify this assumption by the following lemma.

Lemma 2.1 *Each NTA$_w$can be converted into an equivalent NTA$_w$without useless states in polynomial time.*

Proof An NTA$_w$ $B = (\Sigma, Q, \delta, F)$ can be converted into an equivalent NTA$_w$ without useless states in polynomial time as follows:

(1) Compute the set E of states q such that $L(B_q) = \emptyset$.
(2) Replace every occurrence of a symbol in E in all regular expressions in the definition of δ by $\emptyset$ and remove all symbols of E from Q and F.
(3) In the resulting NTA$_w$, compute the set U of states that are not reachable from a state in F.
(4) Remove all states of U from all regular expressions in the definition of δ and remove them from Q.

We note that this procedure closely follows the procedure that removes useless nonterminals from an extended context-free grammar which was presented in [1,22] and where it is also explained that it can be performed in polynomial time. We note that the ordering between steps (2) and (3) is important. If this ordering is reversed, the algorithm does not remove all useless states from the NTA$_w$ with $F = \{q_0\}$ and transition function defined as $\delta(q_0,a) = q_1 q_2$, $\delta(q_1,a) = q_1$, and $\delta(q_2,a) = \varepsilon$. □

Since useless states can be removed efficiently, we also do not need to bother about removing useless states in the NTA$_w$s we construct in our algorithms.

The proof of the following theorem is a straightforward reduction to and from the finite alphabet case [35]. To represent the automata as used in [35], we use the same structure as for NTA$_w$s. We call the latter *NTAs without wildcards*, and their semantics is just as for NTA$_w$s, except that $\diamond$ is given no special meaning. That is, $\diamond$ is allowed in Σ, and the rule (2.2) is not used.

Theorem 2.2 *1. Deciding equivalence of NTA$_w$s is EXPTIME-complete.*
2. Deciding universality of NTA$_w$s is EXPTIME-complete.

Proof We prove the EXPTIME upper bound for equivalence and the EXPTIME lower bound for universality. Since an NTA$_w$ is universal if and only if it is equivalent to some (fixed) NTA$_w$ that accepts $\mathscr{T}_\Delta$, the whole theorem follows.

We first show that equivalence is in EXPTIME. Let N_1 and N_2 be two NTA$_w$s over alphabet Σ_1 and Σ_2, respectively. In particular, let $N_1 = (\Sigma_1, Q_1, \delta_1, F_1)$ and $N_2 = (\Sigma_2, Q_2, \delta_2, F_2)$. Notice that Σ_1 might be different from Σ_2. We define two NTAs (without wildcards) M_1 and M_2 over the alphabet $\Gamma = \Sigma_1 \cup \Sigma_2 \cup \{\diamond\}$ as follows. The automaton $M_1 = (\Gamma, Q_1, \delta_1', F_1)$ has the following transitions for each $q \in Q_1$ and $\sigma \in \Gamma$:

1. if $\sigma \in \Sigma_1 \cup \{\diamond\}$, then $\delta_1'(q,\sigma) = \delta_1(q,\sigma)$, and
2. if $\sigma \in \Sigma_2 - \Sigma_1$, then $\delta_1'(q,\sigma) = \delta_1(q,\diamond)$.

The automaton $M_2 = (\Gamma, Q_2, \delta_2', F_2)$ and δ_2' are defined similarly.

We want to show that M_1 is equivalent to M_2 (over $\mathscr{T}_\Gamma$) if and only if N_1 is equivalent to N_2 (over $\mathscr{T}_\Delta$). For any tree $t \in \mathscr{T}_\Delta$, let $t_\diamond \in \mathscr{T}_\Gamma$ be the tree obtained from t by replacing the label of any node that is not in $\Sigma_1 \cup \Sigma_2$, with $\diamond$. Since the transitions of N_i and M_i agree on all labels $\sigma \notin \Sigma_1 \cup \Sigma_2$, it holds that for any tree $t \in \mathscr{T}_\Delta$ and run λ on t, λ is an accepting run of N_i on t if and only if it is an accepting run of M_i on $t_\diamond$, for $i \in \{1,2\}$. Let t be a tree in $\mathscr{T}_\Gamma$.

For the *only if* direction, suppose that $t \in L(N_1)$. Then there exists an accepting run λ of N_1 on t. By construction of M_1, λ is also an accepting run of M_1 on $t_\diamond$, and hence $t_\diamond \in L(M_1)$. By assumption that M_1 and M_2 are equivalent, there is an accepting run λ' of M_2 on $t_\diamond$. By construction of M_2, λ' is also an accepting run of N_2 on any tree t' which is such that $t'_\diamond = t_\diamond$. Hence, λ' is also an accepting run of N_2 on t. The case is similar when $t \in L(N_2)$.

For the *if* direction, suppose that $t \in L(M_1)$. Then there is an accepting run λ of M_1 on t. Then, by construction of M_1, the run λ is an accepting run of N_1 on any tree t' which is such that $t'_\diamond = t$. By assumption that N_1 and N_2 are equivalent, it holds that $t' \in L(N_2)$, with λ' being the witness accepting run, and by construction of M_2, λ' is an accepting run of M_2 on $t'_\diamond = t$. The case is similar when $t \in L(M_2)$.

We continue by showing EXPTIME-hardness of universality. Let N be an NTA without wildcards over alphabet Σ. Then let M be an arbitrary but fixed NTA$_w$ over the alphabet Σ which accepts any tree containing at least one symbol from $\Delta - \Sigma$. In other words, M accepts exactly the trees in $\mathscr{T}_\Delta - \mathscr{T}_\Sigma$. The NTA$_w$ M requires only two states that are not states of N. Then N is universal over Σ if and only if $N \cup M$ is universal over Δ. □

2.3 Queries

The focus of this paper is on unary queries. Basically, a unary query maps each tree to a subset of its nodes.

Definition 2.3 (Unary Query) A *unary query* $\mathscr{Q}$ is a mapping with domain $\mathscr{T}_\Delta$ that is closed under isomorphism, and is such that for each $t \in \mathscr{T}_\Delta$, $\mathscr{Q}(t) \subseteq \mathsf{Nodes}^t$.

For two unary queries $\mathscr{Q}, \mathscr{Q}'$, and $\odot \in \{\subseteq, \supseteq, =\}$, we write $\mathscr{Q} \odot \mathscr{Q}'$ if, for all $t \in \mathscr{T}_\Delta$, we have $\mathscr{Q}(t) \odot \mathscr{Q}'(t)$. In this paper we only consider unary queries and "query" will therefore mean "unary query".

To facilitate proofs, in the following, we will sometimes reduce unary queries to Boolean ones. To this end, we will employ a standard technique (cf., e.g., [38]) which extends the set of labels by $\Sigma \times \{0,1\}$ and labels selected nodes by 1 and non-selected nodes by 0. We will in the following, without loss of generality, assume that $(\Delta \times \{0,1\}) \subset \Delta$. This assumption simplifies the text in our proofs.

Definition 2.4 For a tree $t \in \mathscr{T}_\Delta$, we denote the set of nodes labelled by a symbol in Σ, as $\mathsf{Nodes}^t(\Sigma)$. Then, let $\mathsf{bool}_\Sigma(\cdot,\cdot)$ be the mapping defined as follows. For each tree $t \in \mathscr{T}_\Delta$ and $v \in \mathsf{Nodes}^t(\Sigma)$, let $\mathsf{bool}_\Sigma(t,v) \in \mathscr{T}_\Delta$ be the tree with the same nodes and edges as t, but with the labelling function defined as follows: $\mathsf{lab}^{\mathsf{bool}_\Sigma(t,v)}(v) = (\mathsf{lab}^t(v), 1)$, for $v' \in \mathsf{Nodes}^t(\Sigma) - \{v\}$, $\mathsf{lab}^{\mathsf{bool}_\Sigma(t,v)}(v') = (\mathsf{lab}^t(v'), 0)$, and for $v' \notin \mathsf{Nodes}^t(\Sigma)$, $\mathsf{lab}^{\mathsf{bool}_\Sigma(t,v)}(v') = \mathsf{lab}^t(v')$. Finally, for a unary query $\mathscr{Q}$, let

$$\mathsf{BoolQ}_\Sigma(\mathscr{Q}) = \bigcup_{\substack{t \in \mathscr{T}_\Delta \\ v \in \mathscr{Q}(t)}} \{\mathsf{bool}_\Sigma(t,v)\}.$$

Then, the image of the function bool_Σ is:

$$\mathsf{Image}(\mathsf{bool}_\Sigma) = \bigcup_{\substack{t \in \mathscr{T}_\Delta \\ v \in \mathsf{Nodes}^t(\Sigma)}} \{\mathsf{bool}_\Sigma(t,v)\}.$$

Lemma 2.5 *For any finite $\Sigma \subseteq \Delta$:*

1. *bool_Σ is injective.*
2. *BoolQ_Σ is injective.*

Proof (1) Let $t_1, t_2 \in \mathscr{T}_\Delta$, $v_1 \in \mathsf{Nodes}^{t_1}$ and $v_2 \in \mathsf{Nodes}^{t_2}$, and assume $\mathsf{bool}_\Sigma(t_1,v_1) = \mathsf{bool}_\Sigma(t_2,v_2)$. The latter implies immediately that t_1 and t_2 have the same nodes and edges, since bool_Σ preserves the structure of the tree. For each node $v \in \mathsf{Nodes}^{t_1}$, since $\mathsf{lab}^{\mathsf{bool}_\Sigma(t_1,v_1)}(v) = \mathsf{lab}^{\mathsf{bool}_\Sigma(t_2,v_2)}(v)$, by definition also $\mathsf{lab}^{t_1}(v) = \mathsf{lab}^{t_2}(v)$. Finally, also $v_1 = v_2$, since otherwise $\mathsf{bool}_\Sigma(t_1,v_1)$ and $\mathsf{bool}_\Sigma(t_2,v_2)$ would have different labels at the nodes v_1 and v_2.

(2) To prove this we reformulate the definition of BoolQ_Σ to get

$$\mathsf{BoolQ}_\Sigma(\mathscr{Q}) = \{\mathsf{bool}_\Sigma(t,v) \mid (t,v) \in \mathscr{Q}\}$$

Assume unary queries $\mathscr{Q}_1$ and $\mathscr{Q}_2$ such that $\mathsf{BoolQ}_\Sigma(\mathscr{Q}_1) = \mathsf{BoolQ}_\Sigma(\mathscr{Q}_2)$. But since bool_Σ is injective this implies that $\mathscr{Q}_1 = \mathscr{Q}_2$. □

Lemma 2.5 implies that the mapping bool_Σ has an inverse over its image. We denote the inverse by $\mathsf{bool}_\Sigma^{-1}$.

2.4 Selecting tree automata

The general formalism we use for expressing unary queries is that of selecting tree automata, which are defined as follows [16,26].

Definition 2.6 (NSTA$_w$) A *non-deterministic selecting tree automaton (with wildcards)* or *NSTA$_w$* M, is a pair (N,S), where N is an NTA$_w$ with state set Q, and $S \subseteq Q$ is a set of *selecting states*. The query defined by M is denoted $\mathscr{Q}_M$. Formally, $v \in \mathscr{Q}_M(t)$ if there is an accepting run λ such that $\lambda(v) \in S$ and $\mathsf{lab}^t(v) \in \Sigma$. Note that for all $t \notin L(N)$, $\mathscr{Q}_M(t) = \emptyset$. The *size* of M is defined as the size of its underlying NTA$_w$.

We refer to the class of queries defined by NSTA$_w$s as the (unary) regular queries. An NSTA$_w$ M is called *non-empty* if there is a t such that $\mathscr{Q}_M(t) \neq \emptyset$.

We say that two NSTA$_w$s are *equivalent* if they define the same query. The following theorem says that deciding equivalence of NSTA$_w$s is in EXPTIME. Although the results seems to belong to folklore, for the sake of completeness, we provide a proof below.

Specifically, Theorem 2.8 follows directly from the following lemma and Theorem 2.2.

Lemma 2.7 *For any finite $\Sigma \subseteq \Delta$ and any NSTA$_w$, $M = (N_M, S)$ over Σ, we can construct in polynomial time an NTA$_w$ N such that $L(N) = \mathsf{BoolQ}_\Sigma(\mathscr{Q}_M)$, and such that $|Q_N| = 2 \cdot |Q_{N_M}|$, where Q_N is the set of states of N and Q_{N_M} is the set of states of N_M.*

Proof Let $N_M = (\Sigma, Q, \delta, F)$. We will construct two NTA$_w$s, N' and N'', such that $L(N'') = \mathsf{Image}(\mathsf{bool}_\Sigma)$, and $L(N') \cap \mathsf{Image}(\mathsf{bool}_\Sigma) = \mathsf{BoolQ}_\Sigma(\mathscr{Q}_M)$. This implies that $\mathsf{BoolQ}_\Sigma(\mathscr{Q}_M) = L(N') \cap L(N'')$. Since the intersection of NTA$_w$s can be done using a cross-product construction, the whole construction can be performed in polynomial time.

The NTA$_w$ $N'' = (\Sigma \times \{0,1\}, \{q_0, q_U\}, \delta'', \{q_0\})$, where for each $a \in \Sigma$,

$$\delta''(q_U,(a,0)) = q_U^*, \delta''(q_0,(a,0)) = q_U^* q_0 q_U^*, \delta''(q_0,(a,1)) = q_U^*,$$

and the wildcard transitions are $\delta''(q_U,\diamond) = q_U^*$ and $\delta''(q_0,\diamond) = q_U^* q_0 q_U^*$. To see that $L(N'') = \mathsf{Image}(\mathsf{bool}_\Sigma)$ note first that N''_{q_U} recognizes all the trees where for each node, there is no $a \in \Sigma$, such that the label is $(a,1)$. The state q_0 can be assigned to a node if it has a label of the form $(a,1)$ for $a \in \Sigma$, or if it is not labelled $(a,1)$, for $a \in \Sigma$, and q_0 is assigned to exactly one of its children, and q_U is assigned to the other nodes. Hence, q_0 is reached at a node if exactly one node in the tree has a label of the form $(a,1)$, where $a \in \Sigma$.

The NTA$_w$ $N' = (\Sigma \times \{0,1\}, Q, \delta', F)$ has δ' defined as follows: for each $a \in \Sigma$ and $q \in Q$, $\delta'(q,(a,0)) = \delta(q,a)$, for each $q \in S$, $\delta'(q,(a,1)) = \delta(q,a)$, and for each $q \in Q$, $\delta'(q,\diamond) = \delta(q,\diamond)$.

We first show that

$$L(N') \cap \mathsf{Image}(\mathsf{bool}_\Sigma) \subseteq \mathsf{BoolQ}_\Sigma(\mathscr{Q}_M)$$

Assume $t' \in L(N') \cap \mathsf{Image}(\mathsf{bool}_\Sigma)$. Let $(t,v) = \mathsf{bool}_\Sigma^{-1}(t')$. Hence $\mathsf{lab}^{t'}(v) = (\mathsf{lab}^t(v), 1)$, while for each $v' \in \mathsf{Nodes}^t(\Sigma) - \{v\}$, $\mathsf{lab}^{t'}(v') = (\mathsf{lab}^t(v'), 0)$. Let λ be the run of N' on t'. By construction, λ is also a run of (Σ, Q, δ, F) on t, and $\lambda(v) \in S$. Hence $v \in \mathscr{Q}_M(t)$, and therefore $\mathsf{bool}_\Sigma(t,v) \in \mathsf{BoolQ}_\Sigma(\mathscr{Q}_M)$, that is, $t' \in \mathsf{BoolQ}_\Sigma(\mathscr{Q}_M)$.

Secondly we show that

$$\mathsf{BoolQ}_\Sigma(\mathscr{Q}_M) \subseteq L(N') \cap \mathsf{Image}(\mathsf{bool}_\Sigma)$$

First note that $\mathsf{BoolQ}_\Sigma(\mathscr{Q}_M) \subseteq \mathsf{Image}(\mathsf{bool}_\Sigma)$, so we only need to show that

$$\mathsf{BoolQ}_\Sigma(\mathscr{Q}_M) \subseteq L(N')$$

Assume $t' \in \mathsf{BoolQ}_\Sigma(\mathscr{Q}_M)$. Let $(t,v) = \mathsf{bool}_\Sigma^{-1}(t')$. Hence, $v \in \mathscr{Q}_M(t)$, $v \in \mathsf{Nodes}^t(\Sigma)$, and there is an accepting run λ of (Σ, Q, δ, F) on t such that $\lambda(v) \in S$. But by construction λ is then also an accepting run of N' on t'.

Finally, since N' has $|Q|$ states and N'' has 2 states the cross product construction defining the intersection of their languages has $2 \cdot |Q|$ states as required. □

Theorem 2.8 *Deciding equivalence of NSTA$_w$s is EXPTIME-complete.*

Proof For the lower bound, by Theorem 2.2 we can reduce the problem of NTA$_w$ equivalence to NSTA$_w$ equivalence. Given any NTA$_w$ N, we convert it to an NSTA$_w$ M with N as its underlying NTA$_w$, that always selects the root of a tree in the language of N.

For the upper bound, given two NSTA$_w$s M_1 and M_2, we construct in polynomial time two NTA$_w$s N_1 and N_2 as in Lemma 2.7, such that $L(N_1) = \mathsf{BoolQ}_\Sigma(\mathscr{Q}_{M_1})$ and $L(N_2) = \mathsf{BoolQ}_\Sigma(\mathscr{Q}_{M_2})$. By Lemma 2.5 $\mathscr{Q}_{M_1} = \mathscr{Q}_{M_2}$ if and only if $\mathsf{BoolQ}_\Sigma(\mathscr{Q}_{M_1}) = \mathsf{BoolQ}_\Sigma(\mathscr{Q}_{M_2})$. By Theorem 2.2, we can check in EXPTIME whether N_1 and N_2 are equivalent. □

3 Regular Path Definability

In this section, we consider regular path definability. Here, we use NFA$_w$s to define regular paths. More precisely, we investigate in Section 3.1 whether a query given by an NSTA$_w$ can already be defined by an NFA$_w$. We further discuss in Section 3.2 the relationship with definability of single-type EDTDs. Finally, we address tractability in Section 3.3.

3.1 NFA$_w$-definability

We first formally introduce queries defined by NFA$_w$s.

Definition 3.1 (NFA$_w$-definable Query) The query defined by an NFA$_w$ A is denoted by $\mathscr{Q}_A$ and is defined as follows. For any tree $t \in \mathscr{T}_\Delta$, $\mathscr{Q}_A(t) = \{v \in \mathsf{Nodes}^t \mid \mathsf{lab}^t(v) \in \Sigma, \mathsf{ancstr}^t(v) \in L(A)\}$. We say that a query $\mathscr{Q}$ is *NFA$_w$-definable*, if there is an NFA$_w$ A such that $\mathscr{Q} = \mathscr{Q}_A$.

As selection of a node only depends on the ancestor-string, NFA_w-definable queries are ancestor-based as defined next:

Definition 3.2 (Ancestor-based Query) A unary query $\mathscr{Q}$ is *ancestor-based* if for each two trees $t_1, t_2 \in \mathscr{T}_\Delta$, and for any nodes $v_1 \in \mathsf{Nodes}^{t_1}$ and $v_2 \in \mathsf{Nodes}^{t_2}$, if $v_1 \in \mathscr{Q}(t_1)$ and $\mathsf{ancstr}^{t_1}(v_1) = \mathsf{ancstr}^{t_2}(v_2)$, then also $v_2 \in \mathscr{Q}(t_2)$.

It is easy to see that each NFA_w-definable unary query must be ancestor-based.

Lemma 3.3 *If a unary query is NFA_w-definable, then it is also ancestor-based.*

Proof Let the unary query $\mathscr{Q}$ be definable by an NFA_w A, i.e., $\mathscr{Q} = \mathscr{Q}_A$, and assume $t_1, t_2 \in \mathscr{T}_\Delta$ such that $v_1 \in \mathscr{Q}(t_1)$, $v_2 \in \mathsf{Nodes}^{t_2}$ and $\mathsf{ancstr}^{t_1}(v_1) = \mathsf{ancstr}^{t_2}(v_2)$. Since $v_1 \in \mathscr{Q}_A(t_1)$, by definition, $\mathsf{ancstr}^{t_1}(v_1) \in L(A)$, and since $\mathsf{ancstr}^{t_1}(v_1) = \mathsf{ancstr}^{t_2}(v_2)$, also $\mathsf{ancstr}^{t_2}(v_2) \in L(A)$, hence, $v_2 \in \mathscr{Q}(t_2)$. □

In general, the converse of Lemma 3.3 does not hold. For example, the query "select all nodes v such that $\mathsf{ancstr}^t(v)$ has an equal number of a's and b's" is ancestor-based but not NFA_w-definable. We will show in the remainder of this section, that ancestor-based *regular* queries do correspond precisely to the NFA_w-definable ones. The proof makes use of a specific construction on NSTA_ws. In particular, for a given NSTA_w M we construct an automaton $\mathsf{NFA}(M)$ such that M is NFA_w-definable iff $\mathscr{Q}_{\mathsf{NFA}(M)} = \mathscr{Q}_M$.

Basically, the automaton $\mathsf{NFA}(M)$ is constructed from M by turning it into an NFA_w. That is, a state at a node is only dependent on the state assigned to its parent (and no longer dependent on the states assigned to its siblings). Specfically, any state in $\mathsf{Labels}(\delta_M(q,a))$ can be assigned to a node whose parent is labelled a and is assigned state q where δ_M is the transition function of M.[2] The formal construction is given next:

Definition 3.4 For an NSTA_w $M = (N, S)$, where $N = (\Sigma, Q, \delta, F)$, and for $q_I \notin Q$, define the NFA_w

$$\mathsf{NFA}(M) = (\Sigma, (Q \times \Sigma_\diamond) \cup \{q_I\}, q_I, \delta', F'),$$

where $\Sigma_\diamond = \Sigma \uplus \{\diamond\}$ and

$$F' = \{(p,a) \mid p \in S, a \in \Sigma_\diamond \text{ and } \delta(p,a) \text{ is defined and not empty}\},$$

for each $a \in \Sigma_\diamond$, let $\delta'(q_I, a) = \{(p,a) \mid p \in F\}$, and for $q \in Q$ and $b \in \Sigma_\diamond$, let

$$\delta'((q,a),b) = \{(p,b) \mid p \in \mathsf{Labels}(\delta(q,a))\}.$$

The query defined by $\mathsf{NFA}(M)$ is always *complete*, that is, it always selects at least the nodes that are selected by M. Furthermore, if the query defined by M is ancestor-based, then we have that $\mathsf{NFA}(M)$ is *sound* as well, i.e., each node selected by $\mathsf{NFA}(M)$ is also selected by M. To facilitate the proofs below, we introduce the notation $\mathsf{lab}^{t,\Sigma}(v)$. If $\mathsf{lab}^t(v) \in \Sigma$, then let $\mathsf{lab}^{t,\Sigma}(v) = \mathsf{lab}^t(v)$. Otherwise, let $\mathsf{lab}^{t,\Sigma}(v) = \diamond$.

[2] Recall that $\mathsf{Labels}(r)$ is the set of symbols occurring in regular expressions r.

Lemma 3.5 *Let M be an NSTA$_w$. Then the following holds:*

1. $\mathscr{Q}_M \subseteq \mathscr{Q}_{\mathsf{NFA}(M)}$*; and,*
2. *if $\mathscr{Q}_M$ is ancestor-based then $\mathscr{Q}_{\mathsf{NFA}(M)} \subseteq \mathscr{Q}_M$.*

Proof (1) Let M and $\mathsf{NFA}(M)$ be as in Definition 3.4. Assume $v \in \mathscr{Q}_M(t)$ for some v and t. We will prove that also $v \in \mathscr{Q}_{\mathsf{NFA}(M)}(t)$. Let $v_1 \cdots v_n$ be the path from the root to v in t. (Hence $v_1 = \mathsf{root}(t)$ and $v_n = v$.) Since $v \in \mathscr{Q}_M(t)$, there is an accepting run λ of M on t which selects v, that is, such that $\lambda(v) \in S$. Let $q_1, \ldots, q_n$ be the states assigned to the nodes $v_1, \ldots, v_n$ by such an accepting run. Hence $q_1 \in F$ and $q_n \in S$. By induction on i, where $1 \leq i \leq n$, we prove that $(q_i, \mathsf{lab}^{t,\Sigma}(v_i)) \in \delta'^*(q_I, \mathsf{ancstr}^t(v_i))$.

- For the base case $i = 1$ it suffices to show that
$$(q_1, \mathsf{lab}^{t,\Sigma}(v_1)) \in \delta'^*(q_I, \mathsf{lab}^t(v_1))$$
But this follows from construction of δ', the extended transition function δ'^*, and that $q_1 \in F$.
- For the induction case where $i > 1$, we can assume, by the induction hypothesis, that
$$(q_{i-1}, \mathsf{lab}^{t,\Sigma}(v_{i-1})) \in \delta'^*(q_I, \mathsf{ancstr}^t(v_{i-1}))$$
and it remains to prove that
$$(q_i, \mathsf{lab}^{t,\Sigma}(v_i)) \in \delta'^*((q_{i-1}, \mathsf{lab}^t(v_{i-1})), \mathsf{lab}^t(v_i))$$
By construction of δ' and δ'^*, this holds if
$$q_i \in \mathsf{Labels}(\delta(q_{i-1}, \mathsf{lab}^{t,\Sigma}(v_{i-1})))$$
The latter holds, since λ is an accepting run.

Since $q_n \in S$ and λ is an accepting run, $(q_n, \mathsf{lab}^{t,\Sigma}(v_n)) \in F'$. This implies $\mathsf{ancstr}^t(v) \in L(\mathsf{NFA}(M))$, and hence $v \in \mathscr{Q}_{\mathsf{NFA}(M)}(t)$.

(2) Let $M = (N, S)$, where $N = (\Sigma, Q, \delta, F)$, and
$$\mathsf{NFA}(M) = (\Sigma, (Q \times \Sigma_\diamond) \cup \{q_I\}, q_I, \delta', F')$$
as in Definition 3.4. Assume that for some tree t and node $v \in \mathsf{Nodes}^t$, $v \in \mathscr{Q}_{\mathsf{NFA}(M)}(t)$. We will show that there exists a tree t' and $v' \in \mathsf{Nodes}^{t'}$, such that $v' \in \mathscr{Q}_M(t')$ and $\mathsf{ancstr}^t(v) = \mathsf{ancstr}^{t'}(v')$. By our assumption that $\mathscr{Q}_M$ is ancestor-based, it will follow that $v \in \mathscr{Q}_M(t)$.

Let $v_1, \ldots, v_n$ be the nodes on the path from the root to v (including the root and v), and let $w = \mathsf{ancstr}^t(v)$. Furthermore, let
$$q_I, (p_1, \mathsf{lab}^{t,\Sigma}(v_1)), \ldots, (p_n, \mathsf{lab}^{t,\Sigma}(v_n))$$
be the states visited by $\mathsf{NFA}(M)$ (in order) when matching w. Specifically, this means $(p_n, \mathsf{lab}^{t,\Sigma}(v_n)) \in F'$, $p_n \in S$, and $p_1 \in F$.

Recall that we have defined $N_p = (\Sigma, Q, \delta, \{p\})$ for $p \in Q$ as the NTA$_w$ N with single final state p. We prove (below) by induction on i, $0 \leq i < n$, that there is a tree $t'_{n-i} \in L(N_{p_{n-i}})$ and a $v'_{n-i} \in \mathscr{Q}_{(N_{p_{n-i}},S)}(t'_{n-i})$ such that $\mathsf{lab}^t(v_{n-i}) \cdots \mathsf{lab}^t(v_n) = \mathsf{ancstr}^{t'_{n-i}}(v'_{n-i})$, and that there is a run of $N_{p_{n-i}}$ on t'_{n-i} where the nodes on the path from the root to v'_{n-i} are assigned the states $p_{n-i}, \ldots, p_n$, respectively.

- The base case $i = 0$ is easy, since we know $p_n \in S$ and $(p_n, \mathsf{lab}^{t,\Sigma}(v_n)) \in F'$, and by construction the latter implies $\delta(p_n, \mathsf{lab}^{t,\Sigma}(v_n))$ is defined. Therefore, there is a tree t'_n with its root labelled with $\mathsf{lab}^t(v_n)$, such that $t'_n \in N_{p_n}$ as required.
- For the induction case, we can by the induction hypothesis assume the statement holds for $i \geq 0$, and we prove it for $i+1 < n$. From the run of $\mathsf{NFA}(M)$ on w we must have that $(p_{n-i}, \mathsf{lab}^{t,\Sigma}(v_{n-i}))$ is in

$$\delta'((p_{n-i-1}, \mathsf{lab}^{t,\Sigma}(v_{n-i-1})), \mathsf{lab}^{t,\Sigma}(v_{n-i}))$$

By definition of the transition function δ', this implies

$$p_{n-i} \in \mathsf{Labels}(\delta(p_{n-i-1}, \mathsf{lab}^{t,\Sigma}(v_{n-i-1}))).$$

In particular, there is a string $w_q = q_1 \cdots p_{n-i} \cdots q_r$, such that

$$w_q \in L(\delta(p_{n-i-1}, \mathsf{lab}^{t,\Sigma}(v_{n-i-1})))$$

Since there are no useless states, for each state q_j other than p_{n-i} in w_q there is a tree s_{q_j} such that $s_{q_j} \in L(N_{q_j})$, and by the inductive hypothesis, there is a tree $t'_{n_i} \in L(N_{p_{n-i}})$ with the required properties. Then let

$$t'_{n-i-1} = \mathsf{lab}^t(v_{n-i-1})(s_{q_1} \cdots t'_{n-i} \cdots s_{q_r}).$$

This tree satisfies the induction hypothesis statement.

Since $\{p_1\} \subseteq F$, it holds that $L(N) \supseteq L(N_{p_1})$, and therefore $v'_1 \in \mathscr{Q}_M(t'_1)$, as required. □

The following lemma relates NFA_w-definability and ancestor-based regular queries.

Lemma 3.6 *For an NSTA_w M, the following are equivalent*

1. *$\mathscr{Q}_M$ is NFA_w-definable;*
2. *$\mathscr{Q}_M$ is ancestor-based; and,*
3. *$\mathscr{Q}_M = \mathscr{Q}_{\mathsf{NFA}(M)}$.*

Proof (1) ⇒ (2) holds by Lemma 3.3.
(2) ⇒ (3) holds by Lemma 3.5.
(3) ⇒ (1) holds by definition of NFA_w-definable query. □

We construct an NSTA_w defining the same query as an NFA_w. We remark that there is a difference of one step between how an NSTA_w and an NFA_w matches an ancestor-string: The path employed by an NFA_w while recognizing a word, is by one longer than the word (first the initial state, then one state for each letter), while the NSTA_w only labels each node with one state. We therefore need to introduce a one step increase in the δ-function. To do this, the constructed NSTA_w employs $(Q \times \Sigma_\diamond)$ for the states. We will prove the construction to be correct in Lemma 3.8.

Definition 3.7 Given an NFA$_w$ $A = (\Sigma, Q, q_i, \delta, F)$ we define the NSTA$_w$

$$\mathsf{NSTA}(A) = ((\Sigma, Q', \delta', F'), S)$$

where $Q' = (Q \times \Sigma_\diamond) \uplus \{q_U\}$, $S = (F \times \Sigma_\diamond)$, $F' = \{(q,a) \mid a \in \Sigma_\diamond, q \in \delta(q_I, a)\}$, and δ' is defined as follows: for each $a \in \Sigma_\diamond$ put $\delta'(q_U, a) = q_U^*$, for each $q \in F$ put $\delta'((q,a),a) = r_q + q_U^*$, and for each $q \in Q - F$, put $\delta'((q,a),a) = r_q$, where

$$r_q = q_U^* \cdot \left(\sum_{b \in \Sigma_\diamond, p \in \delta(q,b)} (p,b) \right) \cdot q_U^*.$$

Lemma 3.8 *For each NFA$_w$ A, $\mathscr{Q}_{\mathsf{NSTA}(A)} = \mathscr{Q}_A$.*

Proof Assume $A = (\Sigma, Q, \delta, q_I, F)$, and $\mathsf{NSTA}(A) = ((\Sigma, Q', \delta', F'), S)$ as in Definition 3.7. We first need an auxiliary result: Note that the value of the transition function $\delta'(q,a)$ for a state $q \in Q'$ and letter $a \in \Sigma_\diamond$ is only defined if $q = q_U$ or $q = (q', a)$ for some $q' \in Q$. Hence, for any valid run λ of $\mathsf{NSTA}(A)$ on a tree t, and any node $v \in \mathsf{Nodes}^t$, either $\lambda(v) = q_U$, or $\lambda(v) = (q, \mathsf{lab}^{t,\Sigma}(v))$ for some state $q \in Q$.

We now proceed to prove that $\mathscr{Q}_{\mathsf{NSTA}(A)} \subseteq \mathscr{Q}_A$. Assume that $t \in \mathscr{T}_\Sigma$ and $v \in \mathscr{Q}_{\mathsf{NSTA}(A)}(t)$, and $\lambda : \mathsf{Nodes}^t \to Q'$ a corresponding run such that $\lambda(v) \in S$. Let $v_1, \ldots, v_n$ be the path starting in the root and ending in v. No node on this path can be mapped to q_U, since no state in S is reachable from q_U. By the result above, there are therefore $q_1, \ldots, q_n \in Q$ such that for $i \in \{1, \ldots, n\}$, $\lambda(v_i) = (q_i, \mathsf{lab}^{t,\Sigma}(v_i))$. We prove by induction on i, $1 \leq i \leq n$, that $q_i \in \delta^*(q_I, \mathsf{ancstr}^t(v_i))$.

- For the base case $i = 1$, note first that $q_I \in \delta^*(q_I, \varepsilon)$. Secondly, since λ is an accepting run, we must have that $(q_1, \mathsf{lab}^{t,\Sigma}(v_1))$ is a final state of the NTA$_w$ in A, and by construction therefore $q_1 \in \delta(q_I, \mathsf{lab}^{t,\Sigma}(v_1))$, i.e., $q_1 \in \delta^*(q_I, \mathsf{ancstr}^t(v_1))$.
- For the induction case where $1 < i \leq n$, assume $q_{i-1} \in \delta^*(q_I, \mathsf{ancstr}^t(v_{i-1}))$. Since λ is an accepting run,

  $$(q_i, \mathsf{lab}^{t,\Sigma}(v_i)) \in \mathsf{Labels}(\delta'((q_{i-1}, \mathsf{lab}^{t,\Sigma}(v_{i-1})), \mathsf{lab}^{t,\Sigma}(v_{i-1})))$$

  By construction of δ', this implies that $q_i \in \delta(q_{i-1}, \mathsf{lab}^{t,\Sigma}(v_i))$, so we have $q_i \in \delta^*(q_I, \mathsf{ancstr}^t(v_i))$.

Since also $\lambda(v) = (q_n, \mathsf{lab}^{t,\Sigma}(v)) \in S$, we get $q_n \in F$, hence A accepts $\mathsf{ancstr}^t(v)$.

Secondly, we prove that $\mathscr{Q}_{\mathsf{NSTA}(A)} \supseteq \mathscr{Q}_A$. Assume $t \in \mathscr{T}_\Sigma$ and $v \in \mathscr{Q}_A(t)$, that is, $\mathsf{ancstr}^t(v) \in L(A)$. Let $v_1, \ldots, v_n$ be the path starting at the root and ending in v, and let $q_I, q_1, \ldots, q_n$ be the states visited by a run that accepts $\mathsf{ancstr}^t(v)$ in A. Define $\lambda : \mathsf{Nodes}^t \to (Q \times \Sigma_\diamond) \cup \{q_U\}$ such that for $v' \notin \{v_1, \ldots, v_n\}$, $\lambda(v') = q_U$, while for $1 \leq i \leq n$, let $\lambda(v_i) = (q_i, \mathsf{lab}^{t,\Sigma}(v_i))$. Since $q_n \in F$, we have that $(q_n, \mathsf{lab}^{t,\Sigma}(v)) \in S$, and therefore we must only show that λ is an accepting run. But this is immediate from the construction of δ': q_U is a universal state, and for $i, 1 \leq i < n$, and $k_1, k_2 \in \mathbb{N}$, the word $(q_U)^{k_1} \cdot (q_{i+1}, \mathsf{lab}^{t,\Sigma}(v_{i+1})) \cdot (q_U)^{k_2}$ is in $L(\delta'((q_i, \mathsf{lab}^{t,\Sigma}(v_i)), \mathsf{lab}^{t,\Sigma}(v_i)))$, while for any $k_3 \in \mathbb{N}$, the word $(q_U)^{k_3}$ is in $L(\delta'(q_n, \mathsf{lab}^{t,\Sigma}(v_n)), \mathsf{lab}^{t,\Sigma}(v_n)))$. Finally, $(q_1, \mathsf{lab}^{t,\Sigma}(v_1))$ is in F' be definition of $\mathsf{NSTA}(A)$, since $q_1 \in \delta(q_I, \mathsf{lab}^{t,\Sigma}(v_1))$. □

We are now ready for the main result of this section:

Theorem 3.9 *Deciding whether for an NSTA$_w$ M, $\mathscr{Q}_M$ is NFA$_w$-definable, is complete for EXPTIME.*

Proof The lower bound follows from a reduction from the universality problem for NTA$_w$s (cf. Theorem 2.2). The reduction takes as input an NTA$_w$ $N = (\Sigma, Q, \delta, F)$ and constructs an NSTA$_w$ $M = (N', S)$ as follows. Let $q_{\text{sel}} \notin Q$ and let a be some symbol in Σ. Then let $N' = (\Sigma, Q \cup \{q_{\text{sel}}\}, \delta \cup \{(q_{\text{sel}}, a) \mapsto (\sum_{p \in F} p)^*\}, \{q_{\text{sel}}\})$ and $S = \{q_{\text{sel}}\}$. We show that $\mathscr{Q}_M$ is NFA$_w$-definable iff $L(N) = \mathscr{T}_\Delta$. The query $\mathscr{Q}_M$ selects the root node in all trees $t = a(t_1, \ldots, t_n)$ where for all $1 \leq i \leq n$, $t_i \in L(N)$. If $L(N) = \mathscr{T}_\Delta$, then $\mathscr{Q}_M$ is obviously NFA$_w$-definable, namely by any NFA$_w$ selecting exactly the first letter in words in $a\Delta^*$. On the other hand, suppose $\mathscr{Q}_M$ is NFA$_w$-definable. By Lemma 3.6, the query is ancestor-based and hence for every tree t' with a root labelled by a, the root of t' is in $\mathscr{Q}_M(t')$. Hence $L(N)$ must be exactly $\mathscr{T}_\Delta$.

It remains to show the upper bound. By Lemmas 3.6 and 3.8, it suffices to test $\mathscr{Q}_M = \mathscr{Q}_{\mathsf{NSTA}(\mathsf{NFA}(M))}$. The construction of $\mathsf{NSTA}(\mathsf{NFA}(M))$ can be done in polynomial time and with polynomial increase in size. By Theorem 2.8 the test can be done in exponential time. □

3.2 Single-type EDTDs

In [23], it was shown that deciding whether an NTA is equivalent to a single-type extended DTD is complete for EXPTIME. As single-type EDTDs have ancestor-based *types*, which are superficially similar to ancestor-based queries as defined here, one might wonder what the relationship with the main result of the present section is. Of course, single-type EDTDs do not define queries or process trees which can have labels from an infinite set, but can easily be adapted to do so. Indeed, we can equip them with a wildcard type as our automata and just designate a set of types as output types. Then, the single-type EDTD *selects* those nodes which are assigned a selecting type. We now informally argue that NFAs are a subset of single-type EDTDs w.r.t. the classes of unary queries they define. Indeed, a given NFA can be converted into an equivalent DFA, which can then be directly used to specify an equivalent single-type EDTD through its characterization as a DFA-based DTD [17, 23].

On the other hand, consider the query which selects the root when it has at least two children. The latter is definable by a single-type EDTD but is not NFA-definable as the query is not ancestor-based. To summarize, queries defined by single-type EDTDs can take the branching structure of the tree into account as the formalism is grammar-based, but at the same time type-assignment, and therefore selection, has to be deterministic whereas NFA-definable queries allow for nondeterministic selection but their expressiveness is restricted to single branches. In conclusion, Theorem 3.9 does not seem to imply or follow directly from the corresponding result on single-type EDTDs in [23].

3.3 Tractability

The EXPTIME-hardness in Theorem 3.9 is solely due to the expressiveness of the NSTA$_w$s. Indeed, when M as constructed in the proof is indeed equivalent to an NFA$_w$, that NFA$_w$ is very simple: it just selects the root of the input tree. This means that, even for extremely simple subclasses of XPath (say, linear XPath), deciding definability of NSTA$_w$s within that class remains hard for EXPTIME. To obtain a tractability result we therefore need to restrict the class of regular unary queries. In this regard, Lemma 3.6 and Lemma 3.5 provide already sufficient criteria for tractability. Indeed, any subclass $\mathscr{M}$ of the regular unary queries (or any representation $\mathscr{M}$ of the regular unary queries) for which deciding $\mathscr{Q}_{\mathsf{NFA}(M)} \subseteq \mathscr{Q}_M$ is in PTIME for every $M \in \mathscr{M}$, renders the NFA$_w$-definability problem tractable. The latter is for instance the case for the single-type EDTDs as discussed in the previous section.

4 Twig-definability of NSTA$_w$s

In this section, we address twig-definability of NSTA$_w$s. We start by introducing the necessary definitions for twigs including the concept of characteristic tree in Section 4.1. In Section 4.2, we consider succinctness. In particular, we show that twigs can be exponentially more succinct than NSTA$_w$s and vice versa. This means that we cannot simply guess a small (i.e., polynomially bounded) twig equivalent to a given NSTA$_w$. Fortunately, the exponentially large twigs contain redundancy which can be represented succinctly by folding them into directed acyclic graphs (DAGs). We show in Section 4.3, that when an NSTA$_w$ is equivalent to a twig its DAG-representation is at most of linear size. We further show in Section 4.4 that equivalence of NSTA$_w$s and folded twigs can be tested in exponential time through a reduction to emptiness of alternating tree-walking automata. In Section 4.5, we then obtain our main result, stating that testing twig-definability of NSTA$_w$s is EXPTIME-complete.

4.1 Basics

We start by defining twigs:

Definition 4.1 (Twig Pattern) A *twig pattern*, or simply *twig* is a tuple $T = (\Sigma, t, o, \mathrm{Anc})$, where Σ is a finite subset of Δ, t is a labelled tree over Σ, $\mathrm{Anc} \subseteq \mathsf{Edges}^t$ is the set of *ancestor edges*, and $o \in \mathsf{Nodes}^t$ is a designated output node.

We say that T is a twig *over the alphabet* Σ. The semantics of twigs, however, is always defined over Δ-trees. Formally, an *embedding* of T on a tree s is a total mapping m from Nodes^t to Nodes^s such that

- the root of t is mapped to the root of s,
- $\mathsf{lab}^t(v) = \mathsf{lab}^s(m(v))$, for all $v \in \mathsf{Nodes}^t$, and
- for every two nodes $v_1, v_2 \in \mathsf{Nodes}^t$
  - if $(v_1, v_2) \in \mathsf{Edges}^t - \mathrm{Anc}$, then $(m(v_1), m(v_2)) \in \mathsf{Edges}^s$;
  - if $(v_1, v_2) \in \mathrm{Anc}$, then $m(v_1)$ is an ancestor of $m(v_2)$.

The *language* defined by T is denoted $L(T)$ and consists of all Δ-trees s for which there is an embedding of T into s. The *query* defined by T, denoted by $\mathcal{Q}_T$, is the function that maps a tree s to the set of nodes $v \in \mathsf{Nodes}^s$ for which there is an embedding m of T into s for which $m(o) = v$. In Figure 4.1 we give an example of a twig and an embedding.

Definition 4.2 (Subtwig) For a twig $T = (\Sigma, t, o, \mathrm{Anc})$ and a node $v \in \mathsf{Nodes}^t$, let $T[v]$ be the *subtwig* rooted at v, that is,

$$T[v] = (\Sigma, \mathsf{subtree}^t(v), o, \mathrm{Anc} \cap \{\mathsf{Edges}^{\mathsf{subtree}^t(v)}\})$$

We will use the following basic property of subtwigs.

Lemma 4.3 *For a twig $T = (\Sigma, t, o, Anc)$, a tree $s \in L(T)$, and an embedding m of T into s, $\mathsf{subtree}^s(m(v)) \in L(T[v])$ for every $v \in \mathsf{Nodes}^t$.*

Proof The embedding m is easily modified (by restricting the domain) to an embedding of $T[v]$ into $\mathsf{subtree}^s(m(v))$. □

Definition 4.4 Two twigs T and T' are *language-equivalent* if $L(T) = L(T')$. They are *query-equivalent* if $\mathcal{Q}_T = \mathcal{Q}_{T'}$.

Definition 4.5 (Twig-Definable Query) A unary query $\mathcal{Q}$ is called *twig-definable* if there is a twig T such that $\mathcal{Q} = \mathcal{Q}_T$. A tree language L is called *twig-definable* if there is a twig T such that $L = L(T)$.

Next, we define a tree $c_x(T)$ which is characteristic for a twig T. Basically, the tree is obtained by replacing each ancestor-edge with a sequence of two child edges where the new node is labeled with $x \notin \Sigma$. This tree is a member of the language defined by the twig. In addition, for a twig T', when $c_x(T) \in L(T')$ then $L(T) \subseteq L(T')$. The notion of characteristic trees is similar to the notion of canonical models defined by Miklau and Suciu [25] where every ancestor edge is replaced by a sequence of wildcards. Our notion is simpler because our twigs are less complex than the tree patterns used by Miklau and Suciu. Concretely, the tree patterns of Miklau and Suciu had nodes labeled by wildcards, which our twigs have not.

Definition 4.6 (The Characteristic Tree) For a twig $T = (\Sigma, t, o, \mathrm{Anc})$ and x a label not in Σ, *the characteristic tree* $c_x(T)$ of T is obtained from t by replacing all edges $e = (v_1, v_2)$ in Anc with a path v_1, v_e, v_2 of length 2, with labels $\mathsf{lab}^t(v_1)$, x and $\mathsf{lab}^t(v_2)$, respectively. Here, for every edge e, v_e is a new node occurring nowhere else in $c_x(T)$.

So, if $T = (\Sigma, t, o, \mathrm{Anc})$, every node $v \in \mathsf{Nodes}^t$, corresponds to a unique node of the tree $c_x(T)$. And every node in $c_x(T)$ not labelled x corresponds to a unique node in t. Hence, the identity over Nodes^t is a bijection between Nodes^t and the nodes in $c_x(T)$ not labelled x. We denote by id^t this identity function on Nodes^t. Lemma 4.7 shows that id^t is an embedding and we will refer to it as the *canonical embedding* from T into its characteristic tree. Figure 4.1 illustrates $c_x(T)$ and id^t.

Lemma 4.7 *For any twig $T = (\Sigma, t, o, Anc)$ and $x \notin \Sigma$, the identity id^t is:*

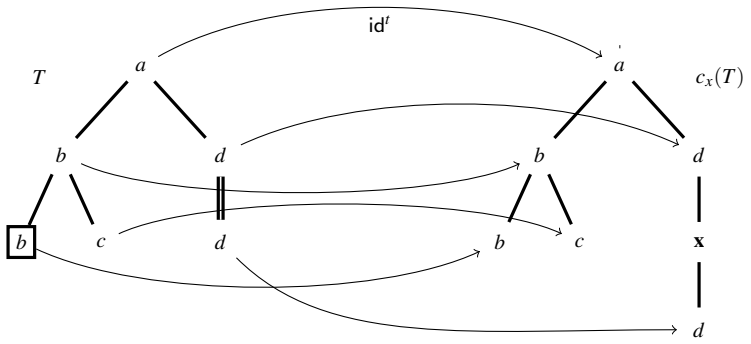


Figure 4.1 A twig $T = (\Sigma, t, o, \mathrm{Anc})$ on the left, its characteristic tree $c_x(T)$ on the right and the canonical embedding id^t. Edges of the twig in Anc are depicted as double edges and o is depicted with a rectangle.

- *an embedding of T into $c_x(T)$*
- *a bijective function between Nodes^t and the set of all nodes in $c_x(T)$ not labelled x.*

Proof We first show that id^t is an embedding of T in $c_x(T)$. This is shown by an induction on the height of t. The base case where t has one node v is immediate, since then also $c_x(T)$ has one node, with the same label $\mathsf{lab}^t(v)$. For the induction case, assume that the statement holds for all trees of height no more than K, for some $K \in \mathbb{N}$. Assume then that t is of height $K+1$. The root r of t is mapped to the root r of $c_x(T)$. For each child v of the root, where $(r,v) \notin \mathrm{Anc}$, (r,v) is also an edge in $c_x(T)$, and is such that $\mathsf{subtree}^{c_x(T)}(v) = c_x(T[v])$. If $(r,v) \in \mathrm{Anc}$, r has in $c_x(T)$ a child labelled x which has v as a single child, again such that $\mathsf{subtree}^{c_x(T)}(v) = c_x(T[v])$. By the induction hypothesis the statement holds for the subtrees $c_x(T[v])$ for each child v of r in t and therefore id^t is an embedding of T on $c_x(T)$.

The identity is of course a bijection. We only need to assert that the nodes labelled x in $c_x(T)$ are exactly those not in t. The latter follows from the construction in Definition 4.6. Since the identity is its own inverse we will not introduce any new notation for the inverse of id^t. □

We will often use the following observation in our proofs.

Remark 4.8 For every $v \in \mathsf{Nodes}^t$, $\mathsf{subtree}^{c_x(T)}(v) = c_x(T[v])$.

The next lemma states that all embeddings and the inverses of all canonical embeddings preserve the ancestor relation. Its proof is immediate from the definitions.

Lemma 4.9 *For a twig $T = (\Sigma, t, o, Anc)$ and two nodes $u, v \in \mathsf{Nodes}^t$:*

- *if u is an ancestor of v in t then for any tree $s \in L(T)$, and embedding m of T on s, $m(u)$ is an ancestor of $m(v)$ in s.*
- *if u is an ancestor of v in $c_x(T)$, then u is also an ancestor of v in t.*

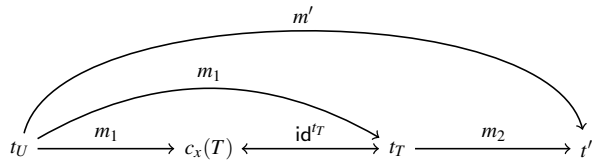


Figure 4.2 The relation between the mappings and trees used in the proof of Lemma 4.10

The proof of the following lemma is similar to the proof of Proposition 3 of [25].

Lemma 4.10 *For any two twigs T,U over an alphabet Σ with $x \notin \Sigma$, $c_x(T) \in L(U)$ implies $L(T) \subseteq L(U)$.*

Proof Let $T = (\Sigma, t_T, o_T, \mathrm{Anc}_T)$ and $U = (\Sigma, t_U, o_U, \mathrm{Anc}_U)$, and m_1 the embedding of U on $c_x(T)$. To prove that $L(T) \subseteq L(U)$, we assume a tree $t' \in L(T)$, and prove $t' \in L(U)$. Let m_2 be an embedding of T on t'. Since the image of m_1 consists of nodes in $c_x(T)$ not labelled x, which by Lemma 4.7 is exactly the nodes of t_T, we can compose m_1 with m_2. We will show that this composed mapping, $m' = m_2 \circ m_1$, is an embedding of U on t'. The composition of m' is illustrated in Fig. 4.2.

It remains to show that the conditions for an embedding given in Definition 4.1 hold for m'. Recall first that for $v \in \mathsf{Nodes}^{t_U}$, $m_1(v)$ is not labelled x, hence $m_1(v)$ is in Nodes^{t_T} and has the same label as v. The two first properties of Definition 4.1, namely mapping of the root and preservation of labels, therefore carry over easily from the same properties of m_1 and m_2. For the last property, let $(v_1, v_2) \in \mathsf{Edges}^{t_U}$. If $(v_1, v_2) \notin \mathrm{Anc}_U$, then, since m_1 is an embedding onto $c_x(T)$, $(m_1(v_1), m_1(v_2)) \in \mathsf{Edges}^{c_x(T)}$. From the construction of a characteristic tree, Def. 4.6, we therefore get $(m_1(v_1), m_1(v_2)) \in \mathsf{Edges}^{t_T} - \mathrm{Anc}_T$. Finally, from m_2 being an embedding of T on t' we therefore get $(m'(v_1), m'(v_2)) \in \mathsf{Edges}^{t'}$. On the other hand, if $(v_1, v_2) \in \mathrm{Anc}_U$, then, since m_1 is an embedding onto $c_x(T)$, $m_1(v_1)$ is an ancestor of $m_1(v_2)$ in $c_x(T)$. By Lemma 4.9 $m_1(v_1)$ is then also an ancestor of $m_1(v_2)$ in t_T. Further, from m_2 being and embedding and applying Lemma 4.9 once more, $m'(v_1)$ is an ancestor of $m'(v_2)$ in t'. Hence, m' is an embedding of U onto t' and $t' \in L(U)$. □

We conclude this section with showing that the characteristic tree of a (proper) subtwig is not in the language of the whole twig.

Lemma 4.11 *For a twig $T = (\Sigma, t, o, Anc)$ and a non-root node $v \in \mathsf{Nodes}^t$,*

$$c_x(T[v]) \notin L(T)$$

Proof Let $v_1, \ldots, v_n$ be the n nodes on the longest path in t. Since v_1 is the root of t, and hence $v_1 \notin \mathsf{Nodes}^{\mathsf{subtree}^t(v)}$, all paths in $\mathsf{subtree}^t(v)$ have less than n nodes. Hence all paths in $c_x(T[v])$ have less than n nodes with label different from x. Any embedding of T on $c_x(T[v])$ must map the nodes $v_1, \ldots, v_n$ to distinct nodes, each an ancestor of the next, on the same path, none labelled x. As no such path exists in $c_x(T[v])$, there cannot be any embedding of T on $c_x(T[v])$. □

A useful corollary is that the language of the subtwig cannot be completely included in the language of the whole twig:

Corollary 4.12 *For a non-root node v of a twig T, $L(T[v]) \not\subseteq L(T)$.*

4.2 Succinctness and minimality

Next, we discuss succinctness and minimality of twigs. The *size* of a twig T, denoted by $|T|$, is defined as the number of nodes in its underlying tree. We distinguish two kinds of minimality.

Definition 4.13 (Minimal twig) A twig is *language-minimal* (resp., *query-minimal*) if there is no language-equivalent (resp., query-equivalent) twig of strictly smaller size.

The following lemma summarizes basic facts on minimality used in this paper.

Lemma 4.14 *1. If a twig is language-minimal, then it is also query-minimal.*
2. *There are query-minimal twigs which are not language-minimal.*
3. *If a twig $T = (\Sigma, t, o, Anc)$ is query-minimal, then for all $v \in \mathsf{Nodes}^t$ where $o \notin \mathsf{Nodes}^{\mathsf{subtree}^t(v)}$, the twig $T[v]$ is language-minimal.*
4. *If $T = (\Sigma, t, o, Anc)$ is a language-minimal twig, then for all nodes $v \in \mathsf{Nodes}^t$, $T[v]$ is also language-minimal.*

Proof 1. Assume a twig T is language-minimal. For any twig T' such that $\mathscr{Q}_T = \mathscr{Q}_{T'}$ it must be the case that $L(T) = L(T')$, so T' cannot be smaller than T.

2. Let $T = (\Sigma, t, o, \mathrm{Anc})$, where t consists of three nodes: one root node having two child nodes. Furthermore, all labels are ℓ. Let o be one of the leaves, and let the edge from the root to o be in Anc. Now, $L(T)$ is all trees where the root and at least one child of the root is labelled ℓ. Further, $\mathscr{Q}_T$ selects any non-root node labelled ℓ in a tree in $L(T)$. T is not language-minimal, since the node o and the edge in Anc could be removed from the tree without affecting the recognized language. But T is query-minimal. If it was not, there should be a twig $T' = (\Sigma, t', o', \mathrm{Anc}')$ with two nodes, one the child of the other, and with the leaf being the node o'. In both cases where the edge does or does not belong in Anc$'$, the twig is not query equivalent to T.
3. By contradiction: If $T[v]$ is not language-minimal, then T is not query-minimal, since the smaller twig that is language-equivalent to $T[v]$, can replace $T[v]$ also in T.
4. By an immediate contradiction: if $T[v]$ is not language-minimal, then the smaller twig that is language-equivalent to $T[v]$, can be used at position v in T to give a smaller twig recognizing $L(T)$.
   In particular, let $v \in \mathsf{Nodes}^t$ and suppose $T' = (\Sigma, t', o', \mathrm{Anc}')$ is a language-minimal twig and is such that $L(T') = L(T[v])$. Suppose for contradiction that T' has less nodes than $T[v]$. We want to show that for any tree $t_1 \in L(T)$, there is an embedding m' from $T[v \leftarrow T'] = (\Sigma, t'', o'', \mathrm{Anc}'')$ to t_1. Let m_1 be the embedding from T to t_1 and let m_2 be the embedding from T' to $\mathsf{subtree}^{t_1}(m_1(v))$.

Notice that $\mathsf{context}^t(v) = \mathsf{context}^{t''}(v)$ and $\mathsf{subtree}^{t''}(v) = t'$. Define m' as

$$m'(v') = \begin{cases} m_1(v') \text{ if } v' \in \mathsf{Nodes}^{\mathsf{context}^{t''}(v)} \\ m_2(v') \text{ if } v' \in \mathsf{Nodes}^{\mathsf{subtree}^{t''}(v)} \end{cases}.$$

Then, m' preserves the labelling of the nodes and the child and ancestor edges, both over the disjoint domains $\mathsf{Edges}^{\mathsf{context}^{t''}(v)}$ and $\mathsf{Edges}^{\mathsf{subtree}^{t''}(v)}$, and the edge not in $\mathsf{Edges}^{\mathsf{context}^{t''}(v)} \cup \mathsf{Edges}^{\mathsf{subtree}^{t''}(v)}$. Therefore m' is an embedding from $T[v \leftarrow T']$ to t_1, which is a contradiction to T being language-minimal. □

Twig-minimality plays an important role in the technical machinery developed in the next section. The following lemma specifies two sufficient criteria for a twig not to be language minimal.

Lemma 4.15 *For a twig $T = (\Sigma, t, o, Anc)$, x a label not in Σ, and two edges (v, v') and (v, v'') in t with $v' \neq v''$, then T is not language-minimal when either of the following conditions holds:*

- $(v, v'') \notin Anc$ *and* $c_x(T[v'']) \in L(T[v'])$*; or,*
- $(v, v') \in Anc$ *and* $\exists u \in \mathsf{Nodes}^{\mathsf{subtree}^t(v'')} : c_x(T[u]) \in L(T[v'])$.

Moreover, $\mathsf{subtree}^t(v')$ *can be removed from the twig without affecting the recognized language.*

Proof We assume one of the two statements holds, and show that $\mathsf{subtree}^t(v')$ can be removed from t without affecting the language recognized by the twig. This leads to a twig $T' = (\Sigma, t', o', \mathrm{Anc}')$ with at least one less node. Note first that $L(T) \subseteq L(T')$, since any embedding of T is easily modified into an embedding of T', by restricting the domain of the embedding. It remains to show that $L(T') \subseteq L(T)$. Let $t_1 \in L(T')$ and m_1 an embedding of T' on t_1. We show $t_1 \in L(T)$ by a case distinction:

In the first case we have $(v, v'') \notin \mathrm{Anc}$ and $c_x(T[v'']) \in L(T[v'])$. Since the subtrees at v' and v'' have no common nodes we have that $T'[v''] = T[v'']$, and therefore $c_x(T'[v'']) = c_x(T[v''])$. Since $c_x(T[v'']) \in L(T[v'])$, we have that $c_x(T'[v'']) \in L(T[v'])$. By applying Lemma 4.10 we therefore get $L(T'[v'']) \subseteq L(T[v'])$. By Lemma 4.3,

$$\mathsf{subtree}^{t_1}(m_1(v'')) \in L(T'[v'']) \text{ and } \mathsf{subtree}^{t_1}(m_1(v'')) \in L(T[v'])$$

Let m_2 be an embedding of $T[v']$ on $\mathsf{subtree}^{t_1}(m_1(v''))$. Notice that $m_2(v') = m_1(v'')$, as the root of $T[v']$ must be mapped to the root of $\mathsf{subtree}^{t_1}(m_1(v''))$, which is $m_1(v'')$.

Define the mapping $m' : \mathsf{Nodes}^t \to \mathsf{Nodes}^{t_1}$ as follows. For all $u \in \mathsf{Nodes}^t$,

$$m'(u) = \begin{cases} m_1(u) \text{ if } u \in \mathsf{Nodes}^{\mathsf{context}^t(v')} \\ m_2(u) \text{ if } u \in \mathsf{Nodes}^{\mathsf{subtree}^t(v')} \end{cases}$$

We want to show that m' is an embedding of T on t_1. By definition m' preserves the labelling of the nodes, and over the disjoint domains $\mathsf{Edges}^{\mathsf{context}^t(v')}$ and

$\mathsf{Edges}^{\mathsf{subtree}^t(v')}$, the mapping m' preserves child and ancestor edges. For the edge $(v,v') \notin \mathsf{Edges}^{\mathsf{context}^t(v')} \cup \mathsf{Edges}^{\mathsf{subtree}^t(v')}$, it holds that

$$(m'(v), m'(v')) = (m_1(v), m_2(v')) = (m_1(v), m_1(v''))$$

is an edge in t_1, since $(v,v'') \notin \text{Anc}$. Therefore, m' is an embedding of T on t_1, irrespective of whether $(v,v') \in \text{Anc}$ or $(v,v') \notin \text{Anc}$ in t.

In the other case, $(v,v') \in \text{Anc}$ and $u \in \mathsf{Nodes}^{\mathsf{subtree}^t(v'')}$, such that $c_x(T[u]) \in L(T[v'])$. Since the subtrees at u and v' are non-overlapping, we have $c_x(T[u]) = c_x(T'[u])$, hence $c_x(T'[u]) \in L(T[v'])$. By Lemma 4.10, $L(T'[u]) \subseteq L(T[v'])$, and by Lemma 4.3 $\mathsf{subtree}^{t_1}(m_1(u)) \in L(T'[u])$. Therefore, $\mathsf{subtree}^{t_1}(m_1(u)) \in L(T[v'])$. Let m_2 be an embedding of $T[v']$ on $\mathsf{subtree}^{t_1}(m_1(u))$. Notice that $m_2(v') = m_1(u)$, since the root of $T[v']$ must be mapped by m_2 to the root of $\mathsf{subtree}^{t_1}(m_1(u))$.

Define the mapping $m' : \mathsf{Nodes}^t \to \mathsf{Nodes}^{t_1}$ as follows. For all $z \in \mathsf{Nodes}^t$,

$$m'(z) = \begin{cases} m_1(z) \text{ if } z \in \mathsf{Nodes}^{\mathsf{context}^t(v')} \\ m_2(z) \text{ if } z \in \mathsf{Nodes}^{\mathsf{subtree}^t(v')} \end{cases}$$

We want to show that m' is an embedding of T on t_1. Firstly, notice that by definition, m' preserves the labelling of the nodes. Furthermore, over the disjoint domains $\mathsf{Edges}^{\mathsf{context}^t(v')}$ and $\mathsf{Edges}^{\mathsf{subtree}^t(v')}$, m' preserves child and ancestor edges. For the edge $(v,v') \notin \mathsf{Edges}^{\mathsf{context}^t(v')} \cup \mathsf{Edges}^{\mathsf{subtree}^t(v')}$, notice that $m'(v) = m_1(v)$ and $m'(v') = m_2(v')$ by the definition of m', and therefore $m'(v)$ is an ancestor of $m'(v')$, since $m_2(v') = m_1(u)$, and $m_1(v)$ is an ancestor of $m_1(u)$. □

Using Lemma 4.15, we can now show that for a minimal twig, the canonical embedding is the only embedding on the characteristic tree.

Lemma 4.16 *For a language-minimal twig $T = (\Sigma, t, o, Anc)$, there is exactly one embedding of T into $c_x(T)$.*

Proof Let m be an embedding from T to $c_x(T)$ which is different from the canonical embedding id^t. Then, let v_1 be a node in t of minimum height (closest to the root), such that $v_1 \neq m(v_1)$, and let v be the parent of v_1 in t. Note that no node of t can be mapped by any embedding to a node labelled with x in $c_x(T)$, and therefore let $v_2 \in \mathsf{Nodes}^t$ be such that $v_2 = m(v_1)$. Notice also that by Definition 4.1 m must map the root of t to the root of $c_x(T)$, and therefore v_1 is not the root.

We want to show that v_1 cannot be mapped to $m(v_1)$. From the embedding m and Remark 4.8, we have

$$\mathsf{subtree}^{c_x(T)}(m(v_1)) = \mathsf{subtree}^{c_x(T)}(v_2) = c_x(T[v_2]),$$

and by our assumption that m is an embedding from T to $c_x(T)$, by Lemma 4.3 we have that $\mathsf{subtree}^{c_x(T)}(m(v_1)) \in L(T[v_1])$, and hence $c_x(T[v_2]) \in L(T[v_1])$. Therefore, by Lemma 4.10, $L(T[v_2]) \subseteq L(T[v_1])$.

We consider two cases, one where v_2 is a child of v, and one where it is simply a descendant of v. Consider the first case. By our assumption that T is language-minimal, the conditions of Lemma 4.15 cannot be satisfied, and hence, if $(v,v_1) \in$

Anc then by the second condition of the lemma, $c_x(T[v_2]) \notin L(T[v_1])$. Similarly, if $(v,v_2) \notin \text{Anc}$, by the first condition of the lemma, we have again that $c_x(T[v_2]) \notin L(T[v_1])$. Therefore, $(v,v_2) \in \text{Anc}$ and $(v,v_1) \notin \text{Anc}$. But, $m(v_1) = v_2$, and therefore, since $(v,v_2) \in \text{Anc}$, $m(v_1)$ cannot be a child of v in $c_x(T)$, as there is an additional node between v and v_2 labelled x. This contradicts the fact that $(v,v_1) \notin \text{Anc}$, and hence m violates the conditions for being an embedding.

Consider then the second case where v_2 is a descendant of v in t, and suppose firstly that v_2 is not a descendant of v_1. Then, let v_2' be the ancestor of v_2 that is a sibling of v_1 in t, but different from v_1. The twig T is language-minimal and therefore the conditions of Lemma 4.15 are not satisfied. Therefore, by the second condition of the lemma, if $(v,v_1) \in \text{Anc}$ there exists no node $u \in \mathsf{Nodes}^{\mathsf{subtree}^t(v_2')}$ such that $c_x(T[u]) \in L(T[v_1])$. In particular, this contradicts $c_x(T[v_2]) \in L(T[v_1])$, and therefore the edge (v,v_1) must not be in Anc. But then m is not a valid embedding, since $m(v_1) = v_2$ is not a child of $m(v) = v$ in $c_x(T)$.

Finally, consider the case where v_2 is a descendant of v_1 in addition to being a descendant of v. But by Lemma 4.11, the node v_2 cannot be a descendant of v_1, since $c_x(T[v_2]) \in L(T[v_1])$, which is a contradiction. □

We conclude our discussion on minimality with the following lemma. By construction it always holds that $c_x(T) \in L(T)$ for $x \notin \Sigma$. Assume T is minimal and let u be one of its nodes. When we replace the subtree rooted at node u in $c_x(T)$ by a new tree t' resulting in the tree $s = c_x(T)[u \leftarrow t']$, then the lemma says that when s still happens to be in the language defined by T then $T[u]$, the twig rooted at u, can always be mapped somewhere in t'.

Lemma 4.17 *Let x be a label not in Σ. For a language-minimal twig $T = (\Sigma, t, o, Anc)$ over Σ, a node $u \in \mathsf{Nodes}^t$, and a tree $t' \in \mathscr{T}_\Delta$, if $c_x(T)[u \leftarrow t'] \in L(T)$, then there is a node $u' \in \mathsf{Nodes}^{t'}$ such that $\mathsf{subtree}^{t'}(u') \in L(T[u])$.*

Proof Let $t'' = c_x(T)[u \leftarrow t']$ and suppose that $t'' \in L(T)$. Then, there is an embedding m of T on t''. Note first that $u \notin \mathsf{Nodes}^{t''}$, since it is replaced by $\mathsf{root}(t')$. Further, by Definition 4.1, for $v' \in \mathsf{Nodes}^{\mathsf{context}^t(u)}$, $m(v')$ is either in $\mathsf{Nodes}^{t'}$ or in $\mathsf{Nodes}^{\mathsf{context}^{t''}(u)} - \{u\}$. The latter case is equal to $m(v') \in \mathsf{Nodes}^{\mathsf{context}^t(u)} - \{u\}$, since $\mathsf{context}^{t''}(u) = \mathsf{context}^{c_x(T)}(u)$, and $x \notin \Sigma$. We will show that $m(u)$ can be the u' in the lemma. That is, we will show that $\mathsf{subtree}^{t'}(m(u)) \in L(T[u])$. It suffices to prove that $m(u) \in \mathsf{Nodes}^{t'}$. We show a slightly stronger statement by induction on the path from the root to u in t. For each node v on the path, either

1. $m(v) \in \mathsf{Nodes}^{t'}$; or,
2. $m(v)$ is on the path from v to u in t.

The base case is the root $\mathsf{root}(t)$. If $u = root(t)$, then $m(\mathsf{root}(t)) = \mathsf{root}(t')$ and the first part of the induction hypothesis holds. Otherwise, by Definitions 4.1 and 4.6 $m(\mathsf{root}(t)) = \mathsf{root}(t)$, and the second condition of the induction hypothesis holds.

For the induction case, assume $v \in \mathsf{Nodes}^t$ is the lowest node in the path in t from the root to u for which the induction hypothesis has been shown to hold. If the first statement holds, then it also holds for the children of v, and we are done. Otherwise,

$m(v)$ is on the path from v to u in t. Let v_1 be the child of v on the path from v to u in t. If $m(v_1) \in \mathsf{Nodes}^{t'}$ or if $v_1 = m(v_1)$ we are done, since then the first or the second statement, respectively, holds. Otherwise, that is, if $m(v_1) \notin \mathsf{Nodes}^{t'}$ and $v_1 \neq m(v_1)$, we treat separately the cases where the edge between v and v_1 is or is not in Anc.

Suppose first that the edge (v, v_1) is not in Anc. This means, by definition of embeddings, that $m(v_1)$ is a child of $m(v)$ in t''. By the construction of $c_x(T)$, $m(v_1)$ is therefore also a child of $m(v)$ in t. We now treat separately the two cases depending on whether $m(v) = v$.

If $m(v) = v$, then $m(v_1) \neq v_1$ is a sibling of v_1 in t, while v_1, and therefore not $m(v_1)$, is an ancestor of u, by definition of the canonical embedding. But then $\mathsf{subtree}^{t''}(m(v_1)) = \mathsf{subtree}^{c_x(T)}(m(v_1))$, and the latter is equal to $c_x(T[m(v_1)])$ by Remark 4.8. By Lemma 4.3, and the embedding m, $\mathsf{subtree}^{t''}(m(v_1)) \in L(T[v_1])$ and therefore $c_x(T[m(v_1)]) \in L(T[v_1])$. Furthermore, v_1 and $m(v_1)$ are siblings and $(v, v_1) \notin$ Anc and $(v, m(v_1)) \notin$ Anc. By Lemma 4.15, this contradicts our assumption that T is language-minimal.

Since $m(v) = v$ leads to a contradiction, we have $m(v) \neq v$. From the induction hypothesis we then get that $m(v)$ is a descendant of v in t. Since v_1 and $m(v)$ both are on the path from v to u we get that $m(v_1)$ is either on the path from v_1 to u, or is a sibling of a node on the path from v_1 to u. In the last case, notice that $\mathsf{subtree}^{t''}(m(v_1)) = \mathsf{subtree}^{c_x(T)}(m(v_1))$, which in turn is equal to $c_x(T[m(v_1)])$, by Remark 4.8. By Lemma 4.3 and the embedding m, $\mathsf{subtree}^{t''}(m(v_1)) \in L(T[v_1])$. It follows that $c_x(T[m(v_1)]) \in L(T[v_1])$. But $T[v_1]$ is a language-minimal twig, and $m(v_1)$ is a descendant of v_1, and by Lemma 4.11 this is a contradiction. Therefore $m(v_1)$ is on the path from v_1 to u, and the induction hypothesis holds for v_1.

Consider now the case where $(v, v_1) \in$ Anc. We remind the reader that $v_1 \neq m(v_1)$, $m(v_1) \notin \mathsf{Nodes}^{t'}$ and the second condition of the inductive hypothesis holds for v. That is, $m(v) \notin \mathsf{Nodes}^{t'}$. Note that $m(v_1)$ is a descendant of $m(v)$ also in t. Let v_3 be the child of $m(v)$ and ancestor of (or equal to) $m(v_1)$ in t.

We prove by contradiction that the second statement of the induction hypothesis holds. That is, we assume that $m(v_1)$ is not on the path from v_1 to u in t, and show that this leads to contradiction. From the latter assumption, we get that $\mathsf{subtree}^{t''}(m(v_1))$ does not contain t'. Therefore, since $\mathsf{context}^{t''}(u) = \mathsf{context}^{c_x(T)}(u)$, we get

$$\mathsf{subtree}^{t''}(m(v_1)) = \mathsf{subtree}^{c_x(T)}(m(v_1)).$$

By Remark 4.8 $\mathsf{subtree}^{c_x(T)}(m(v_1)) = c_x(T[m(v_1)])$. Combining the two latter equalities we get

$$\mathsf{subtree}^{t''}(m(v_1)) = c_x(T[m(v_1)]). \tag{4.1}$$

By applying Lemma 4.3 to T, m, t'' and v_1 it holds that $\mathsf{subtree}^{t''}(m(v_1)) \in L(T[v_1])$. Combining the latter with (4.1) we get

$$c_x(T[m(v_1)]) \in L(T[v_1]). \tag{4.2}$$

Now, $m(v)$ is on the path from v to u by the inductive hypothesis, and we consider the two cases where $m(v) \neq v$ and $m(v) = v$. In the first case, $m(v)$ is a descendant

of v, and therefore v_3 and $m(v_1)$ are descendants of v_1. By Lemma 4.11, it holds that $c_x(T[m(v_1)]) \notin L(T[v_1])$, which contradicts (4.2). In the case where $m(v) = v$, v_3 is either equal to v_1 or a sibling of v_1. If $v_3 = v_1$, $m(v_1)$ is a descendant of v_1 and a similar argument using Lemma 4.11 as above, leeds to a contradiction. If v_3 is a sibling of v_1, we have from Lemma 4.15, the fact that $(v, v_1) \in \text{Anc}$, and our assumption that T is language-minimal, that for any descendant of v_3, and therefore in particular $m(v_1)$ as well, $c_x(T[m(v_1)]) \notin L(T[v_1])$, which also contradicts (4.2).

We have shown that assuming that $m(v_1)$ is not on the path from v_1 to u in t leads to a contradiction. Therefore the induction hypothesis holds for v_1 also in the case where $(v, v_1) \in \text{Anc}$. □

Next, we discuss succinctness of twigs and NSTAs.

Theorem 4.18 *1. There is a family of NSTAs M_n (for $n \in \mathbb{N}$) of size $\mathcal{O}(n)$ such that the smallest query-equivalent twig is of size $\Omega(2^n)$.*
2. For every twig T of size n, there exists an equivalent NSTA of size $\mathcal{O}(2^n)$.
3. There is a family of twigs T_n (for $n \in \mathbb{N}$) of size $\mathcal{O}(n)$ such that the smallest query-equivalent NSTA is of size $\Omega(2^n)$.

Proof (1) First, we define a few more notions regarding subtrees that will be referred to in what follows. If S is a subset of Nodes^t, we say that S is connected if, for every two nodes $v_1, v_2 \in S$, there is a node v and paths from v to v_1 and to v_2 using only nodes in S. Notice that v may be equal to v_1 or v_2. For a tree t and a connected subset S of Nodes^t, the *subgraph t' of t induced by S*, is the tree with $\mathsf{Nodes}^{t'} = S$ and $\mathsf{Edges}^{t'} = (S \times S) \cap \mathsf{Edges}^t$.

Fix the alphabet $\Sigma = \{a, b\}$. For each $n \in \mathbb{N}$, we define the NSTA $M_n = ((\Sigma, Q_n, \delta_n, F_n), F_n)$, $Q_n = \{q_u, q_0, q_{1,a}, q_{1,b}, \ldots, q_{n,a}, q_{n,b}\}$, $F_n = \{q_0\}$, and δ_n is defined as follows. For $1 \leq i < n$, and $\sigma \in \Sigma$

$$\begin{aligned}
\delta_n(q_{i,\sigma}, \sigma) &= (q_u^* \cdot q_{i+1,a} \cdot q_u^* \cdot q_{i+1,b} \cdot q_u^*) + (q_u^* \cdot q_{i+1,b} \cdot q_u^* \cdot q_{i+1,a} \cdot q_u^*), \\
\delta_n(q_{n,\sigma}, \sigma) &= q_u^*, \\
\delta_n(q_0, a) &= (q_u^* \cdot q_{1,a} \cdot q_u^* \cdot q_{1,b} \cdot q_u^*) + (q_u^* \cdot q_{1,b} \cdot q_u^* \cdot q_{1,a} \cdot q_u^*), \\
\delta_n(q_u, \sigma) &= q_u^*, \\
\delta_n(q_u, \diamond) &= q_u^*.
\end{aligned}$$

For each $n \in \mathbb{N}$, let S'_n be the set of complete binary trees of height n, where the root is labelled with a and each non-leaf node has exactly two children, one labelled with a and one with b. Then $\mathcal{Q}_{M_n}$ contains exactly the pairs $(s, \mathsf{root}(s))$ where s has an induced subgraph s' such that $s' \in S'_n$ and $\mathsf{root}(s) = \mathsf{root}(s')$.

Assume, for the purpose of proving a contradiction, that the twig T'_n has less than $2^n - 1$ nodes and is such that $\mathcal{Q}_{T'_n} = \mathcal{Q}_{M_n}$. Let $s' \in S'_n$ and m be the embedding of T'_n on s'. By the pidgeon-hole principle, there must be a node $v \in \mathsf{Nodes}^{s'}$ which is not in the image of m. Let s_{err} be the same as s' except that we change the label of v. m is now obviously also an embedding of T'_n on s_{err}, but $s_{err} \notin \mathcal{Q}_{M_n}$. This contradicts our assumption that $\mathcal{Q}_{T'_n} = \mathcal{Q}_{M_n}$.

(2) We prove by induction on the size n of the twig $T = (\Sigma, t, o, \text{Anc})$, that there is an equivalent NSTA M of size $\mathcal{O}(2^n)$ and an NTA N of size $\mathcal{O}(2^n)$ such that $L(N) = L(T)$.

As the base case, suppose that $T = (\Sigma, t, o, \mathrm{Anc})$ is such that t has only one node. Then the NSTA M requires two states, one of them final, to check that the root of the tree is labelled with the same label as the root of t. The set of selecting states S contains just the final state. The NTA N is defined exactly the same, but does not have the set of selecting states.

For the induction case, suppose that for every $m < n$, the statement holds for every twig of size m. Let $T = (\Sigma, t, o, \mathrm{Anc})$ be of size n, and in particular, let $t = a(t_1, \ldots, t_k)$, where the size of t_i is m_i, for all $1 \leq i \leq n$. Hence, $n = 1 + \Sigma_{i=1}^{n} m_i$. We make a first case distinction, depending on whether $o = \mathsf{root}(t)$ or not.

If $o = \mathsf{root}(t)$ then, by the induction hypothesis, for $1 \leq i \leq k$, there exist NTAs N_i, of size $\mathscr{O}(2^{m_i})$, such that $L(N_i) = L(T_i)$, where $T_i = T[v_i]$ and v_i is the root of t_i in t. Denote $T_i = (\Sigma, t_i, o, \mathrm{Anc}_i)$. Then consider the twigs $T_i' = (\Sigma, a(t_i), o, \mathrm{Anc}_i')$, where Anc_i' contains all edges from Anc_i. Furthermore, if the edge between the root of $a(t_1, \ldots, t_n)$ and t_i is in Anc, we also add the edge between the root of $a(t_i)$ and the root of t_i in Anc_i'. We now have that, for each $i = 1, \ldots, n$, there exists an NTA N_i' which has at most two more states than N_i: one state for testing whether the root is labelled a and one state for simulating the ancestor edge between $\mathsf{root}(a(t_i))$ and $\mathsf{root}(t_i)$ in Anc_i', if present. Altogether, the size of N_i' is $\mathscr{O}(2^{m_i} + 2) = \mathscr{O}(2^{m_i})$ such that $L(N_i') = L(T_i')$.

Observe that the product $N = N_1 \times \cdots \times N_k$ for the intersection of these NTAs accepts precisely the language $L(T)$. Furthermore, the size of N is $\mathscr{O}(2^{m_1} \cdots 2^{m_k}) = \mathscr{O}(2^{m_1 + \ldots + m_k}) = \mathscr{O}(2^n)$. Finally, the NSTA M is obtained from N by defining the set of selecting states S to be the accepting states from N.

The construction for the case where o is not the root node of t is analogous. The difference is that we need to deal with the t_j that contains the node o. For this t_j, we take the NSTA $M_j = (N_j, S)$ from the induction hypothesis and adapt it for the twig T_j', similarly as we did for the N_i'. Finally, the NSTA M is then $((N_1 \times \cdots \times N_k), S')$, where $S' = \{(q_1, \ldots, q_k) \mid q_j \in S\}$.

(3) For $n \in \mathbb{N}$, let $\Sigma_n = \{a, a_1, \ldots, a_n\}$ and let $T_n = (\Sigma, t_n, \mathsf{root}(t_n), \mathrm{Anc})$ be the twig where $t_n = a(a_1, \ldots, a_n)$ and $\mathrm{Anc} = \mathsf{Edges}^{t_n}$. For each n, T_n contains $n+1$ nodes, and the trees in $L(T_n)$ are exactly the trees s such that $\mathsf{lab}^s(\mathsf{root}(s)) = a$ and there are nodes $v_1, \ldots, v_n \in \mathsf{Nodes}^s - \{\mathsf{root}(s)\}$ such that $\mathsf{lab}^s(v_1) = a_1, \ldots, \mathsf{lab}^s(v_n) = a_n$.

For each (non-empty, strict) subset S of $\{a_1, \ldots, a_n\}$, fix an arbitrary tree t_S such that t_S is labelled with exactly the labels from S. That is, for every a_i in S, t_S has a node v_i with $\mathsf{lab}^{t_S}(v_i) = a_i$ and such that t_S has no nodes v with $\mathsf{lab}^{t_S}(v) \notin S$. Furthermore, for every such subset S, denote by $\overline{S}$ the set $\{a_1, \ldots, a_n\} - S$. Notice that, for every S, the tree $a(t_S, t_{\overline{S}}) \in L(T_n)$.

Suppose then for contradiction, that there exists an NSTA M with fewer than $2^n - 2$ states, accepting the language $L(T_n)$. Consider the $2^n - 2$ strict (or proper) and non-empty subsets of $\Sigma_n - \{a\}$, and for each such subset S_i, consider the tree $a(t_{S_i}, t_{\overline{S_i}})$. The NSTA M has an accepting run on each of these trees, and each of these runs assigns some state to the node $\mathsf{root}(t_{S_i})$. By the pigeon hole principle, there must therefore be two different non-empty, strict subsets S_1 and S_2 of $\Sigma_n - \{a\}$, such that on the trees

$$a(t_{S_1}, t_{\overline{S_1}}) \text{ and } a(t_{S_2}, t_{\overline{S_2}}),$$

M has accepting runs λ_1 and λ_2 that assign the same state q to the root of t_{S_1} and the root of t_{S_2}. We can assume w.l.o.g. that $S_2 \not\subseteq S_1$. (If $S_2 \subseteq S_1$ then we can switch S_1 and S_2.) Notice that M also has an accepting run λ on the tree $t = a(t_{S_1}, t_{\overline{S_2}})$. Indeed, this accepting run λ is the same as λ_1 on the subtree t_{S_1}, it is the same as λ_2 on subtree $t_{\overline{S_2}}$ and on the root of t. However, since $S_2 \not\subseteq S_1$, there exists an $a_i \in S_2 - S_1$. As the tree $t = a(t_{S_1}, t_{\overline{S_2}})$ does not contain the label a_i, it is not in $L(T_n)$. This means that M does not accept $L(T_n)$ and is a contradiction. □

4.3 DAG-Twigs

Theorem 4.18(1) excludes the possibility to simply guess an equivalent twig of small size for a given NSTA. Fortunately, as we will show in this section, when an NSTA is equivalent to a twig the latter has a small representation as a directed acyclic graph (DAG).

Below, we use DAGs to represent the trees in twigs. As usual, a DAG G is a directed graph $G = (V, E)$, where V is the set of vertices and $E \subseteq V \times V$ is the set of directed edges, and is such that there is no directed cycle in the graph. Note that we do not consider multi-edges. A DAG G over the alphabet Σ has an associated labelling function $\mathsf{lab}^G : V \to \Sigma$. We assume that all DAGs have exactly one vertex with no incoming edges (called the root and denoted by $\mathsf{root}(G)$) and that they are connected. In what follows, we also refer to the vertices of the DAG as nodes.

For any node $v \in V$, let $\mathsf{clean}^G(v)$ be the DAG obtained from G by removing every node that is not reachable from v. We next recursively define the *unfolding* of G into a tree $\mathsf{unfold}(G)$. When $|V| = 1$, $\mathsf{unfold}(G)$ is a single node with the same label as $\mathsf{root}(G)$. When $|V| > 1$, let $U = \{u \in V \mid (\mathsf{root}(G), u) \in E\}$ and let $u_1 <_U \cdots <_U u_m$ be an arbitrary ordering of the nodes in U. Then, for each $1 \leq k \leq m$, let $G_k = \mathsf{clean}^{G - \{\mathsf{root}(G)\}}(u_k)$. The tree $\mathsf{unfold}(G)$ is then defined as

$$\mathsf{lab}^G(\mathsf{root}(G))(\mathsf{unfold}(G_1), \ldots, \mathsf{unfold}(G_m)).$$

We denote by fold^G the canonical mapping from $\mathsf{Nodes}^{\mathsf{unfold}(G)}$ to V. We say that a tree t is *represented* by a DAG G, if G can be unfolded into t.

Definition 4.19 (Dag-Twig) A *DAG-twig* is a tuple $D = (\Sigma, G, o, \mathrm{Anc})$, where $G = (V, E)$ is a DAG over Σ, the node $o \in V$ is such that there is exactly one path from the root to o in G, and $\mathrm{Anc} \subseteq E$. The *query* defined by D, denoted by $\mathscr{Q}_D$, is the query $\mathscr{Q}_T$ where T is the twig $(\Sigma, \mathsf{unfold}(G), o_G, \mathrm{Anc}_G)$ for which

- $\mathsf{fold}^G(o_G) = o$; and,
- $\mathrm{Anc}_G = \{(v, u) \mid (\mathsf{fold}^G(v), \mathsf{fold}^G(u)) \in \mathrm{Anc}\}$.

We say that the DAG-twig D *represents* the twig T.

Notice that, as there is only one path from the root to o there can only be a unique node o_G for which $\mathsf{fold}^G(o_G) = o$. Furthermore, due to the possibly many ways in which a DAG can be unfolded, there are multiple twigs that are represented by a DAG. However, since all these twigs define the same query, we feel that it is justified to refer to $\mathscr{Q}_D$ as *the* query defined by D.

The next theorem says that if an NSTA$_w$ is twig-definable, there exists an equivalent DAG-twig of at most linear size.

Theorem 4.20 *For an NSTA$_w$ $M = (N, S)$ over an alphabet Σ, if $\mathscr{Q}_M$ is twig-definable, then there exists an equivalent DAG-Twig D over alphabet Σ, with at most $2 \cdot |Q_N|$ nodes, where Q_N is the set of states of N.*

Before we start proving Theorem 4.20, we introduce a definition and some lemmas. Recall that in Definition 2.4 we defined the mappings bool_Σ and BoolQ_Σ and how they reduce unary queries to Boolean ones.

We now expand on this notation to define a similar twig:

Definition 4.21 For a twig $T = (\Sigma, t, o, \mathrm{Anc})$, the twig $\mathsf{BoolT}(T)$ is defined as $(\Sigma \times \{0,1\}, \mathsf{bool}_\Sigma(t,o), o, \mathrm{Anc})$.

In the next lemma, we formulate the similarity between BoolT and BoolQ_Σ more exactly.

Lemma 4.22 *For any twig $T = (\Sigma, u, o, Anc)$,*

$$L(\mathit{BoolT}(T)) \cap \mathit{Image}(\mathit{bool}_\Sigma) = \mathit{BoolQ}_\Sigma(\mathscr{Q}_T)$$

Proof We first show that $\mathsf{BoolQ}_\Sigma(\mathscr{Q}_T) \subseteq L(\mathsf{BoolT}(T)) \cap \mathsf{Image}(\mathsf{bool}_\Sigma)$. Since we have that $\mathsf{BoolQ}_\Sigma(\mathscr{Q}_T) \subseteq \mathsf{Image}(\mathsf{bool}_\Sigma)$ by Definition 2.4, we only need to show that $\mathsf{BoolQ}_\Sigma(\mathscr{Q}_T) \subseteq L(\mathsf{BoolT}(T))$. Let t be a tree in $\mathsf{BoolQ}_\Sigma(\mathscr{Q}_T)$. Hence, we have $t \in \mathsf{Image}(\mathsf{bool}_\Sigma)$ and, by Lemma 2.5, we can let $(t', v) = \mathsf{bool}_\Sigma^{-1}(t)$. By Definition 2.4 this implies that $v \in \mathscr{Q}_T(t')$. From Definition 4.1 we then get $t' \in L(T)$, and that there is an embedding m of T on t' is such that $m(o) = v$. We show that m is also an embedding of $\mathsf{BoolT}(T)$ on t. Recall that, by Definition 2.4, t and t' have the same nodes and edges, as do u and $\mathsf{bool}_\Sigma(u,o)$. Anc is also the same in T and $\mathsf{BoolT}(T)$, so it only remains to show that for all $v \in \mathsf{Nodes}^u$, $\mathsf{lab}^t(m(v)) = \mathsf{lab}^{\mathsf{bool}_\Sigma(u,o)}(v)$. Let $v \in \mathsf{Nodes}^u$. Since m is an embedding of T on t', $\mathsf{lab}^{t'}(m(v)) = \mathsf{lab}^u(v)$. If $\mathsf{lab}^{\mathsf{bool}_\Sigma(u,o)}(v) \notin \Sigma$, then $\mathsf{lab}^{\mathsf{bool}_\Sigma(u,o)}(v) = \mathsf{lab}^u(v)$, and $\mathsf{lab}^{t'}(m(v)) \notin \Sigma$, so $\mathsf{lab}^t(m(v)) = \mathsf{lab}^{t'}(m(v))$ and hence $\mathsf{lab}^t(m(v)) = \mathsf{lab}^{\mathsf{bool}_\Sigma(u,o)}(v)$ holds. For $v = o$, note that $\mathsf{lab}^t(m(o)) = (\mathsf{lab}^{t'}(m(o)), 1)$ and $\mathsf{lab}^{\mathsf{bool}_\Sigma(u,o)}(o) = (\mathsf{lab}^u(o), 1)$, so $\mathsf{lab}^t(m(o)) = \mathsf{lab}^{\mathsf{bool}_\Sigma(u,o)}(o)$ holds. Otherwise, if $v \neq o$, and $\mathsf{lab}^{\mathsf{bool}_\Sigma(u,o)}(v) \in \Sigma$, $\mathsf{lab}^t(m(v)) = (\mathsf{lab}^{t'}(m(v)), 0)$ and $\mathsf{lab}^{\mathsf{bool}_\Sigma(u,o)}(v) = (\mathsf{lab}^u(v), 0)$, hence, $\mathsf{lab}^t(m(v)) = \mathsf{lab}^{\mathsf{bool}_\Sigma(u,o)}(v)$ also in this case.

To show that $L(\mathsf{BoolT}(T)) \cap \mathsf{Image}(\mathsf{bool}_\Sigma) \subseteq \mathsf{BoolQ}_\Sigma(\mathscr{Q}_T)$, assume that $t' \in L(\mathsf{BoolT}(T)) \cap \mathsf{Image}(\mathsf{bool}_\Sigma)$, let m be an embedding of $\mathsf{BoolT}(T)$ on t' and let $(t, v) = \mathsf{bool}_\Sigma^{-1}(t')$. By using similar arguments as in the other case above, we prove that m is also an embedding of T on t, and $v = m(o)$. Hence $v \in \mathscr{Q}_T(t)$, therefore $\mathsf{bool}_\Sigma(t,v) \in \mathsf{BoolQ}_\Sigma(\mathscr{Q}_T)$, that is, $t' \in \mathsf{BoolQ}_\Sigma(\mathscr{Q}_T)$. □

We can now prove that query-minimality is transformed by BoolT into language-minimality.

Lemma 4.23 *If a twig T is query-minimal, then $\mathit{BoolT}(T)$ is language-minimal.*

Proof Let $T = (\Sigma, t, o, \text{Anc})$ be a query-minimal twig, and suppose for contradiction that $\mathsf{BoolT}(T)$ is not language-minimal. Then there exists a twig T' that is smaller than $\mathsf{BoolT}(T)$ and is such that $L(T') = L(\mathsf{BoolT}(T))$. We will show that there exists a twig T'' over alphabet Σ which is of same size as T' and such that $L(T') = L(\mathsf{BoolT}(T''))$. By Lemma 4.22 $\mathsf{BoolQ}_\Sigma(\mathscr{Q}_{T''}) = \mathsf{BoolQ}_\Sigma(\mathscr{Q}_T)$. By applying Lemma 2.5 we then get $\mathscr{Q}_{T''} = \mathscr{Q}_T$. Furthermore, by Definition 2.4 T'' and T' then have the same size, that is, smaller than T. Hence T is not query-minimal which is a contradiction. It remains to show the existence of such a twig T''.

Let $T' = (\Sigma, t', o', \text{Anc}')$. We first show that $t' \in \mathsf{Image}(\mathsf{bool}_\Sigma)$. That is, we must show that there is a node $v \in \mathsf{Nodes}^{t'}$ such that $\mathsf{lab}^{t'}(v) \in \Sigma \times \{1\}$ and that for each $v' \in \mathsf{Nodes}^{t'} - \{v\}$, $\mathsf{lab}^{t'}(v') \in (\Sigma \times \{0\}) \cup (\Delta - \Sigma)$. This is shown applying $L(T') = L(\mathsf{BoolT}(T))$ and Definition 4.1. Note first that there are trees in $L(T')$ with node labels only from $(\Sigma \times \{0,1\}) \cup (\Delta - \Sigma)$, so the node labels in t' must also be from this set. Furthermore, there is exactly one node $v \in \mathsf{Nodes}^{t'}$ such that $\mathsf{lab}^{t'}(v) \in \Sigma \times \{1\}$, since $L(\mathsf{BoolT}(T))$ only contains trees with exactly one such node.

We have now shown that $t' \in \mathsf{Image}(\mathsf{bool}_\Sigma)$, so we can let $(t'', v) = \mathsf{bool}_\Sigma^{-1}(t')$. By Definition 4.21 $\mathsf{BoolT}((\Sigma, t'', v, \text{Anc}')) = (\Sigma, t', v, \text{Anc}')$. The size of T' and $(\Sigma, t', v, \text{Anc}')$ is the same, and by Definition 4.21, $L(T') = L((\Sigma, t', v, \text{Anc}'))$, so we can let $T'' = (\Sigma, t'', v, \text{Anc}')$. □

The remainder of this section is devoted to the proof of Theorem 4.20.

Proof Let D be the smallest DAG-twig representing a query-minimal twig equivalent to M. Notice first that the DAG in D can only have labels from Σ. Otherwise, D would require a label which M cannot test for, and hence M and D could not be equivalent. This means that we can safely replace the alphabet of D with Σ. Let $T = (\Sigma, t, o, \text{Anc})$ be the unfolding of D. Towards a contradiction, assume that the size of D, that is, its number of nodes, is larger than $2 \cdot |Q_N|$ where $N = (\Sigma, Q_N, \delta_N, F_N)$. We will identify two nodes in D which can be merged leading to a strictly smaller DAG-twig which unfolds to a twig of the same size as T and is equivalent to T. In other words, the merged DAG-twig will be equivalent to a query-minimal twig as required to contradict our assumption.

Let $x \notin \Sigma$. Recall that fold^D is the canonical mapping from the nodes of T to the nodes of D witnessing that T is represented by D. Next, we view $M = (N, S)$ and T from the perspective of the languages they define. Specifically, let N_b be the NTA accepting $\mathsf{bool}_\Sigma(\mathscr{Q}_M)$ as is given by Lemma 2.7. Note that N_b has at most $2|Q_N|$ states. Furthermore, let $T_b = \mathsf{BoolT}(T)$ as defined in Definition 4.21. Now, by Lemma 4.23, T_b is language-minimal. The following lemma relates N_b and T_b:

Lemma 4.24 *1.* $L(N_b) \subseteq L(T_b)$*; and,*
2. $c_x(T_b) \in L(N_b)$.

Proof From Lemma 2.7, we have that $L(N_b) = \mathsf{BoolQ}_\Sigma(\mathscr{Q}_M)$. By assumption, the latter is equal to $\mathsf{BoolQ}_\Sigma(\mathscr{Q}_T)$ which is equal to $L(T_b) \cap \mathsf{Image}(\mathsf{bool}_\Sigma)$ by Lemma 4.22.

(1): From the above it follows that $L(N_b) \subseteq L(T_b)$.

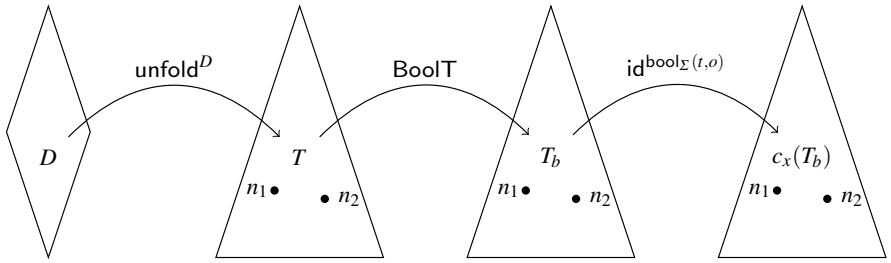


Figure 4.3 The DAG D, the unfolding of D into T, $T_b = \mathsf{BoolT}(T)$, and the characteristic tree of T_b used in the proof of Theorem 4.20.

(2): Notice that $c_x(T_b) \in L(T_b)$ and also $c_x(T_b) \in \mathsf{Image}(\mathsf{bool}_\Sigma)$. Therefore, $c_x(T_b) \in L(N_b)$. □

Let ρ be a run of N_b on $c_x(T_b)$. As N_b has at most $2|Q_N|$ states and D has more than $2|Q_N|$ nodes, by the pigeonhole principle, there are two nodes n_1, n_2 in $c_x(T_b)$, not labelled by x, with $\rho(n_1) = \rho(n_2)$ and corresponding to two different nodes in D. This means, $\mathsf{fold}^D(n_1) \neq \mathsf{fold}^D(n_2)$. Recall that the nodes in $c_x(T_b)$ not labelled x are exactly the nodes in T_b and that $\mathsf{fold}^D(\cdot)$ maps nodes from T to D. Since T_b and T contain the same set of nodes the composition of these two functions is well-defined. Since $\rho(n_1) = \rho(n_2)$, and since $L(N_b) \subseteq L(T_b)$ by Lemma 4.24, it follows that

$$c_x(T_b)[n_1 \leftarrow \mathsf{subtree}^{c_x(T_b)}(n_2)] \in L(T_b), \tag{†}$$

$$c_x(T_b)[n_2' \leftarrow \mathsf{subtree}^{c_x(T_b)}(n_1)] \in L(T_b). \tag{‡}$$

Using (†) and (‡), we can show the following lemma:

Lemma 4.25 *1. $L(T[n_1]) = L(T[n_2])$; and,*
2. neither n_1 nor n_2 is an ancestor of or equal to the output node o.

Before we prove the lemma, let us first explain how it leads to the desired contradiction. From Lemma 4.25(1), it follows that in D the nodes $\mathsf{fold}^D(n_1)$ and $\mathsf{fold}^D(n_2)$ can be *merged* to give a smaller (by at least one node) DAG-twig defining the same query as defined by D. Let $m_1 = \mathsf{fold}^D(n_1)$ and $m_2 = \mathsf{fold}^D(n_2)$. By assumption, $m_1 \neq m_2$. Furthermore, by Corollary 4.12 and Lemma 4.25(1), neither of these nodes can be an ancestor of the other. By merging m_1 and m_2, we mean replacing m_1 with m_2 in all edges of the form (y, m_1) (for any y), removing all edges of the form (m_1, z) (for any z), removing m_1 from the set of nodes, and finally removing all nodes and edges which are now not reachable from the root. Note that this merging is not well-defined when m_1 and m_2 are siblings, because it introduces multi-edges. However, when m_1 and m_2 are siblings then so are n_1 and n_2. But as both $T[n_1]$ and $T[n_2]$ can be embedded on the same subtree of any tree in the language defined by the query, this would mean that T is not query-minimal. Therefore, m_1 and m_2 can not be siblings. Call the thus obtained DAG-Twig D'. Note that by Lemma 4.25(2) there is only one path from the root to the output node o. As D' is equivalent to D, it defines the same query as T, but it still needs to be argued that D' represents a query-minimal twig. That is, the unfolding of D' leads to a twig with the same number of nodes as

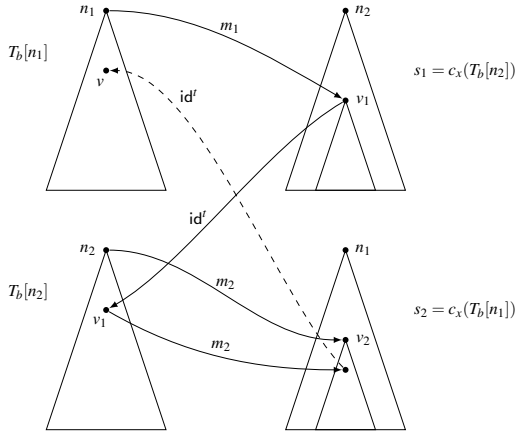


Figure 4.4 Illustration of the trees and associated nodes used in the proof of Lemma 4.25.

T. From Lemma 4.25(2) and Lemma 4.14(3), it follows that both $T[n_1]$ and $T[n_2]$ are language minimal which means that they have the same number of nodes. So, the unfolding of D has the same number of nodes as T and is therefore query-minimal. This leads to the desired contradiction and ends the proof of Theorem 4.20. □

We now prove Lemma 4.25.

Proof Let

$$s_1 = \mathsf{subtree}^{c_x(T_b)}(n_2) \text{ and } s_2 = \mathsf{subtree}^{c_x(T_b)}(n_1).$$

Then, $s_1 = c_x(T_b[n_2])$ and $s_2 = c_x(T_b[n_1])$, by Remark 4.8. To show that $L(T[n_1]) = L(T[n_2])$, we first apply Lemma 4.17 to (†) and (‡), to obtain nodes $v_1 \in \mathsf{Nodes}^{s_1}$ and $v_2 \in \mathsf{Nodes}^{s_2}$ such that

$$\begin{aligned} &\mathsf{subtree}^{s_1}(v_1) \in L(T_b[n_1]), \\ &\mathsf{subtree}^{s_2}(v_2) \in L(T_b[n_2]). \end{aligned} \qquad (\star)$$

Note that, v_1 and v_2 are not labelled with x as the corresponding embeddings map n_1 and n_2 to them. We provide a graphical illustration of the employed trees and associated nodes in Figure 4.4.

If v_1 and v_2 are the roots in the trees s_1 and s_2, respectively, or in other words $v_1 = n_2$ and $v_2 = n_1$, then

$$\mathsf{subtree}^{s_2}(v_2) = \mathsf{subtree}^{s_2}(n_1) = s_2 = c_x(T_b[n_1])$$

Similarly, $\mathsf{subtree}^{s_1}(v_1) = c_x(T_b[n_2])$. Therefore, by $(\star)$,

$$c_x(T_b[n_2]) \in L(T_b[n_1]) \text{ and } c_x(T_b[n_1]) \in L(T_b[n_2]),$$

and by Lemma 4.10, $L(T_b[n_1]) = L(T_b[n_2])$ which implies $L(T[n_1]) = L(T[n_2])$.

Suppose then that at least one of v_1 and v_2 is not the root, and w.l.o.g. let this be the case for v_2. Then we will argue towards a contradiction. Let the mapping m_1 be the embedding showing that $\mathsf{subtree}^{s_1}(v_1) \in L(T_b[n_1])$ and m_2 the embedding showing $\mathsf{subtree}^{s_2}(v_2) \in L(T_b[n_2])$. Consider then the composition of mappings $m = m_2 \circ m_1$. The mapping m is an embedding from $T_b[n_1]$ to $\mathsf{subtree}^{s_2}(m_2(v_1))$. Since v_1 is equal to or a descendant of n_2, so is $m_2(v_1)$ equal to or a descendant of $m_2(n_2)$, and the latter is equal to v_2, because m_2 is the embedding witnessing that $\mathsf{subtree}^{s_2}(v_2) \in L(T_b[n_2])$. As we remarked above, $s_2 = c_x(T_b[n_1])$. So, $\mathsf{subtree}^{s_2}(m_2(v_1)) = c_x(T_b[v])$ where $v = m_2(v_1)$, which is a strict descendant of n_1, by our assumption that v_2 is a strict descendant of n_1. This implies that the mapping m is a witness to $c_x(T_b[v]) \in L(T_b[n_1])$, for v a strict descendant of n_1, and by Lemma 4.11, this leads to a contradiction.

To show that neither n_1 nor n_2 is an ancestor of or equal to o, suppose for contradiction that at least one of them is. If exactly one of them is an ancestor of or equal to o, say n_1, then $T_b[n_1]$ contains a node labelled with $(a,1)$ for some $a \in \Sigma$, but $T_b[n_2]$ does not contain such a node, by definition of the mapping bool_Σ. Therefore $L(T_b[n_1]) \neq L(T_b[n_2])$, which is a contradiction. If both n_1 and n_2 are ancestors of or equal to o, then, either n_1 is an ancestor of n_2, or n_2 is an ancestor of n_1. If n_1 is an ancestor of n_2, and $L(T_b[n_1]) = L(T_b[n_2])$, we have a contradiction by Corollary 4.12. The case is similar when n_2 is an ancestor of n_1.

Hence, $L(T_b[n_1]) = L(T_b[n_2])$ and neither n_1 nor n_2 is an ancestor of or equal to o. Then $L(T[n_1]) = L(T[n_2])$, as needed. □

4.4 Testing equivalence of DAG-Twigs and NSTA$_w$s

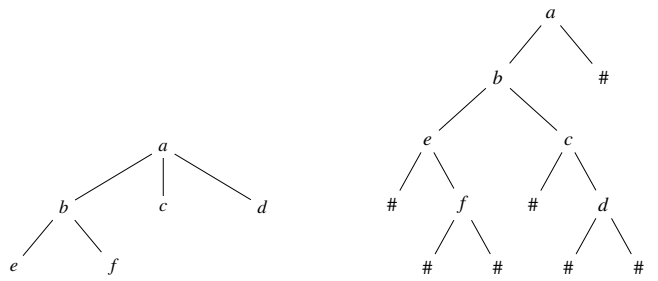
Now that we have a small model property of DAG-twigs compared to NSTA$_w$s (Theorem 4.20), we can simply decide twig-definability of an NSTA$_w$ by guessing the DAG-twig and testing equivalence. Here, we argue that equivalence of such an NSTA$_w$ M and a DAG-twig D can be decided in exponential time. In particular, we will reduce the latter problem to emptiness of alternating tree-walking automata operating on $\mathsf{BoolQ}_\Sigma(\mathscr{Q}_M)$ and $\mathsf{BoolQ}_\Sigma(\mathscr{Q}_D)$.

Let D be a DAG-twig representing the twig T. The goal of this Section is to describe a procedure that, given D, constructs an alternating tree-walking automaton accepting $L(T)$, the tree language associated with T.

Although DAG-twigs operate directly on unranked trees, we will intermediately work with binary trees encoding these unranked trees. Following [27], for an (unranked) tree t, let $\mathsf{enc}(t)$ be its binary encoding, obtained as follows: The nodes of $\mathsf{enc}(t)$ are the nodes of t plus a set of leaf nodes marked #. Further, the root node of $\mathsf{enc}(t)$ is the root node of t and for any node, its left child in $\mathsf{enc}(t)$ is its first child in t (or # if its a leaf), and its right child in $\mathsf{enc}(t)$ is its next sibling in t (or # if it has none). In Figure 4.5, we depicted an example of an unranked tree and its binary encoding.

We start by recalling the definition of these alternating tree walking automata, which operate on binary trees:

Definition 4.26 (Alternating Tree-Walking Automata) Let PosBool(P) be the set of positive Boolean formulas over propositions P (i.e., formulas without negation),



(a) Unranked tree t. (b) Its binary encoding $\mathsf{enc}(t)$.

Figure 4.5 An unranked tree and its binary encoding.

but including true and false. An *alternating tree walking automaton with wildcards* (ATWA with wildcards) over binary trees is defined as a tuple $W = (Q, \Sigma, \delta, q_0)$, where

- Q is a finite set of states,
- Σ is a finite set of alphabet symbols,
- δ is a set of transition rules of the form $(q, \sigma) \to \theta$, where $q \in Q, \sigma \in \Sigma_\diamond$, and θ is a formula from
$$\mathrm{PosBool}(\{\swarrow, \searrow, -\} \times Q),$$
and
- q_0 is the initial state.

Recall that $\Sigma_\diamond = \Sigma \uplus \{\diamond\}$, where $\diamond$ is the wildcard symbol.

The transition relation δ should be such that for each pair $(q, \sigma) \in Q \times \Sigma_\diamond$ there is at most one rule in δ with (q, σ) as its left hand side. (If there would be two rules with the same left hand side, we can merge them into one rule by taking the disjunction of the right hand sides.) If $(q, \sigma) \to \theta \in \delta$, we also write $\mathrm{rhs}_W(q, \sigma) = \theta$. Elements in $\{\swarrow, \searrow, -\}$ denote directions in the tree. For a node u of t, $u \cdot \searrow$ (respectively, $u \cdot \swarrow$) denotes the right child of u (respectively, left child of u) if $\mathrm{lab}(u) \neq \#$ and is undefined otherwise. Further, $u \cdot -$ is u itself (i.e., $-$ is used for stay transitions).

Given a binary tree t, a *run tree* of W on t is an unranked tree R in which each node is labelled by an element of $\mathsf{Nodes}^t \times Q$ such that the following holds. We say that an element $a \in \Delta$ *matches* $\sigma \in \Sigma_\diamond$ if either $a = \sigma$ or $a \notin \Sigma$ and $\sigma = \diamond$.

- The label of the root of R is $(\mathsf{root}(t), q_0)$ and
- for every node x of R with label (v, q_v), if $(q_v, \sigma) \to \theta \in \delta$ and $\mathrm{lab}^t(v)$ matches σ, then there is a set $S \subseteq \{\swarrow, \searrow, -\} \times Q$ such that,
  - for every $(i, q') \in S$, $v \cdot i$ is defined and there is a child y of x in R labelled $(v \cdot i, q')$;
  - all children of x are labelled with $(v \cdot i, q')$ such that $(i, q') \in S$; and
  - the truth assignment that assigns true to all elements of S, and false to all other elements of $\{\swarrow, \searrow, -\} \times Q$, satisfies θ.

A run tree R is *accepting* if, for every leaf node of R labelled (u, q), there is a rule $\mathrm{rhs}_W(q, \sigma) = \mathsf{true}$ such that $\mathrm{lab}^t(u)$ matches σ. A binary tree t is *accepted* by an

For every $a \in \Sigma$, we have the following transitions.
If $u \in V$

and Out-Edges$(u) \neq \emptyset$: $\mathrm{rhs}_W(q_u, a) = \begin{cases} \mathsf{false} & \text{if } \mathrm{lab}^D(u) \neq a, \\ \bigwedge_{e \in \text{Out-Edges}(u)} (-, q_e) & \text{otherwise} \end{cases}$

and Out-Edges$(u) = \emptyset$: $\mathrm{rhs}_W(q_u, a) = \begin{cases} \mathsf{false} & \text{if } \mathrm{lab}^D(u) \neq a, \\ \mathsf{true} & \text{otherwise} \end{cases}$

With $e = (u, v)$,

if $e \notin$ Anc: $\mathrm{rhs}_W(q_e, a) = (\swarrow, q'_e)$
$\mathrm{rhs}_W(q'_e, a) = (-, q_v) \vee (\searrow, q'_e)$

if $e \in$ Anc: $\mathrm{rhs}_W(q_e, a) = (\swarrow, q'_e)$
$\mathrm{rhs}_W(q'_e, a) = (-, q_v) \vee (\swarrow, q'_e) \vee (\searrow, q'_e)$

Figure 4.6 Transitions of the ATWA from the Proof of Lemma 4.27.

ATWA W if there exists an accepting run tree of W on t. By $L(W)$ we denote the set of trees accepted by W.

We now show that, given a DAG-twig, we can efficiently construct an equivalent tree walking automaton. We note that it is well known that there is a connection between various XPath fragments and (two-way) alternating walking automata. Benedikt, Fan and Geerts [3] have shown that it is possible to construct, in linear time, a two-way alternating word automaton, accepting string encodings of trees defined by an XPath query. This construction, however, only works when the considered trees have a fixed depth. Further, ten Cate and Lutz [36] have shown that it is possible to construct, in quadratic time, a two-way alternating tree automaton equivalent to a given XPath query. Our next lemma therefore uses rather standard techniques but, to be complete, we provide the full construction.

Lemma 4.27 *Let D be a DAG-twig representing the twig T. An alternating tree walking automaton W with $L(W) = \{\mathsf{enc}(t) \mid t \in L(T)\}$ can be constructed in time $O(|D|)$.*

Proof Let $D = (\Sigma, G, o, \text{Anc})$ be a DAG-twig and let T be the corresponding unfolded twig. We construct $W = (Q, \Sigma, \delta, q_0)$, such that $L(W) = \{\mathsf{enc}(t) \mid t \in L(T)\}$, as follows. The set Q, contains, for each node u of D, a state q_u and, for each edge e of G, the states q_e and q'_e. A state q_u or q_e can be seen as a pointer to a node u or edge e in the DAG-twig D for which the automaton guesses that the subgraph below u or e, respectively, can be matched at its current position in the tree T. The starting state q_0 is the state corresponding to the root of D.

Finally, the transition relation δ is given in Figure 4.6. (Recall that $\mathrm{rhs}_W(q, a) = \theta$ if and only if $(q, a) \to \theta$ is the unique rule in δ with (q, a) as its left hand side.)

For $G = (V, E)$ and node $u \in V$ let Out-Edges(u) denote the set of outgoing edges of u, i.e., edges of the form (u, v) f for reasons of completeness.or some node v of V. Then, for each node u and each edge $e = (u, v)$ the transitions given in Figure 4.6 apply.

As an example let us look at the transitions from a state corresponding to the ancestor-edge ($e \in$ Anc). At first there is one step to the first child of the current node. From then on, the additional state q'_e is used to search for a proper sibling or descendant node.

It now follows by induction that, for a tree t and $v \in V$, there is an accepting run tree of $W_{q_v} = (Q, \Sigma, \delta, q_v)$ on $\mathsf{enc}(t)$ if and only if, for each node v' of T that corresponds to v, we have $t \in L(T[v'])$.

Finally, it is easy to see that the size of the resulting automaton is linear in the size of D and that it can be computed in linear time. □

The construction for proving Lemma 4.27 can be easily changed such that W accepts encodings of $L(\mathsf{BoolT}(T))$ instead of $L(T)$.

Corollary 4.28 *Let D be a DAG-twig that represents the twig T. An alternating tree walking automaton W with $L(W) = \{\mathsf{enc}(t) \mid t \in L(\mathsf{BoolT}(T))\}$ can be constructed in time $O(|D|)$.*

Proof The proof is almost the same as the one for Lemma 4.27. The only difference is that W needs to make a case distinction between the output node o from D and all other ones. The transition for the output node o then needs to test whether the label of the current node is $(\mathrm{lab}^D(o), 1)$ and all other transitions for nodes u of D test whether the label of the current node is $(\mathrm{lab}^D(u), 0)$. □

We now reduce equivalence between an NSTA$_w$ and a DAG-twig to the emptiness problem for ATWAs.

Theorem 4.29 *Given a DAG-twig D and an NSTA$_w$ M, both over the same alphabet Σ, we can construct an ATWA W in polynomial time such that $L(W) = \emptyset$ if and only if $\mathsf{BoolQ}_\Sigma(\mathscr{Q}_M) = \mathsf{BoolQ}_\Sigma(\mathscr{Q}_D)$.*

Proof Let $D_{0,1} := \mathsf{BoolT}(D)$. Let $N_{0,1}$ be the NTA with $L(N_{0,1}) = \mathsf{BoolQ}_\Sigma(\mathscr{Q}_M)$, as obtained in Lemma 2.7. We construct an ATWA W that accepts a tree t if and only if t is in the symmetric difference of $L(N_{0,1})$ and $L(D_{0,1})$. We assume w.l.o.g. that $D_{0,1}$ and $N_{0,1}$ have disjoint state sets.

When reading a tree t, the ATWA W starts with a stay transition at the root and guesses whether either

- $D_{0,1}$ would accept t and $N_{0,1}$ would reject t; or
- $D_{0,1}$ would reject t and $N_{0,1}$ would accept t.

The ATWA W can do this in one transition:

$$(\mathsf{root}(t), q_0) \to \big((-, q_0^{D_{0,1}}) \wedge (-, \overline{q_0^{N_{0,1}}})\big) \vee \big((-, \overline{q_0^{D_{0,1}}}) \wedge (-, q_0^{N_{0,1}})\big)$$

Here, $q_0^{D_{0,1}}$ and $q_0^{N_{0,1}}$ are the initial states of $D_{0,1}$ and $N_{0,1}$, respectively. The remainder of the run of W starting with $q_0^{D_{0,1}}$ (resp., $q_0^{N_{0,1}}$) therefore leads to acceptance if and only if $D_{0,1}$ (resp., $N_{0,1}$) accepts t. Analogously, the states $\overline{q_0^{D_{0,1}}}$ and $\overline{q_0^{N_{0,1}}}$ are the states for the *complement* languages of $D_{0,1}$ and $N_{0,1}$. The remainder of the run of W starting with $\overline{q_0^{D_{0,1}}}$ (resp., $\overline{q_0^{N_{0,1}}}$) accepts if and only if $D_{0,1}$ (resp., $N_{0,1}$) does *not* accept t. Notice that, since ATWAs can be complemented in polynomial time (analogously to [14], chapter 7), W can be constructed in polynomial time as well. □

Theorem 4.30 *Testing equivalence between a DAG-twig D and an NSTA$_w$ M is EXPTIME-complete.*

Proof The lower bound follows from a reduction from the language universality problem for NTA$_w$s. The latter is EXPTIME-hard by Theorem 2.2. The reduction is similar to that in the proof of Theorem 3.9. It takes as input an NTA$_w$ $N = (\Sigma, Q, \delta, F)$. Let the NSTA$_w$ M and $a \in \Sigma$ be as in the proof of Theorem 3.9. Recall that $\mathscr{Q}_M$ selects the root node in all trees $t = a(t_1, \ldots, t_n)$ where for all $1 \leq i \leq n, t_i \in L(N)$. Let the DAG-twig D have only one node labelled a. Hence, $\mathscr{Q}_M = \mathscr{Q}_D$ if and only if $L(N) = \mathscr{T}_\Delta$.

The upper bound follows from Theorem 4.29, since testing language emptiness for alternating tree walking automata with wildcards is the same as language emptiness for alternating tree walking automata without wildcards, and the latter problem is known to be in EXPTIME. (see, e.g., [7,14]). □

4.5 Main Result

We are now ready to state and prove the main result of this section.

Theorem 4.31 *Deciding whether for an NSTA$_w$ M, $\mathscr{Q}_M$ is twig-definable, is complete for EXPTIME.*

Proof For the lower bound, similarly to Theorem 3.9, we will reduce the problem of universality of NTA$_w$s to the problem considered here. Let $N = (\Sigma, Q, \delta, F)$ be an NTA$_w$. We construct an NSTA$_w$ M such that $\mathscr{Q}_M$ is twig-definable if and only if $L(N) = \mathscr{T}_\Delta$. Let $q_{\text{sel}} \notin Q$ and define the NSTA$_w$ $M = ((\Sigma, Q \uplus \{q_{\text{sel}}\}, \delta \uplus \{(q_{\text{sel}}, a) \mapsto (\sum_{p \in F} p)^*\}), \{q_{\text{sel}}\})$. Then for any tree $t' = a(t_1, \ldots, t_n)$, we have that $\mathsf{root}(t') \in \mathscr{Q}_M(t')$ if and only if, for each $1 \leq i \leq n, t_i \in L(N)$. In particular, we have that $\mathscr{Q}_M$ selects the root of the tree $t_{\text{small}} = a$, consisting of just one node. However, by definition of twig queries, the only twigs that are able to select the root of t_{small} are of the form $(\Sigma', t, o, \text{Anc})$ with $t = a$, $o = \mathsf{root}(t)$, $\text{Anc} = \emptyset$, and $\Sigma' \supseteq \{a\}$. Let $T = (\{a\}, t, o, \text{Anc})$ be such a twig. Then, $\mathscr{Q}_M$ is twig-definable if and only if $\mathscr{Q}_M = \mathscr{Q}_T$. However, $\mathscr{Q}_M = \mathscr{Q}_T$ if and only if $L(N) = \mathscr{T}_\Delta$.

The upper bound is given by the following exponential-time algorithm. From Theorem 4.20, we know that if there exists a DAG-twig equivalent to $M = ((\Sigma, Q, \delta, F), S)$, there is one with alphabet Σ, and that has at most $2 \cdot |Q|$ nodes. Therefore, we can enumerate every possible DAG-twig D with alphabet Σ and at most $2 \cdot |Q|$ nodes and test whether D and M are equivalent. Theorem 4.30 states that we can test in exponential time whether a given DAG-twig D and a given NSTA$_w$ M are equivalent. Since the maximal size of each DAG-twig D is linear in our input, this means that our total algorithm has an exponential-time test for each of the exponentially many DAG-twigs, which takes exponential time altogether. □

5 Conclusion

In this paper we have shown that deciding twig-definability of NSTAs is complete for EXPTIME. There are many possible directions for future work. First of all, it would

be interesting to identify meaningful subclasses of NSTAs for which deciding twig-definability is tractable. On the other hand, one could wonder how twig-queries can be extended while remaining within EXPTIME for testing twig-definability. When an NSTA is not equivalent to a twig, one could look at maximal sub- or minimal super-approximations, as, for instance, done in [17] for single-type EDTDs. Of course, other languages than XPath can be considered, like for instance, the Region Algebra [15], caterpillar expressions [18], or even tree-walking automata [7].

Another interesting question is the complexity of twig-definability in the finite alphabet case. The NSTA$_w$s we consider in this paper have a wildcard symbol. However, what happens if we consider node-selecting tree automata without wildcard? In other words, assume that we have a finite alphabet Σ and we should decide whether a given NSTA (without wildcard transitions) can be rewritten to a twig that returns the same result on every Σ-tree. It seems that this problem requires a different technique than the one we developed here. Lemma 4.10, for instance, does not apply anymore for the simple reason that the construction of the characteristic tree $c_x(T)$ requires a new alphabet symbol x.

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