Monadic Datalog Containment on Trees Using the Descendant-Axis

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Abstract. In their AMW’14-paper, Frochaux, Grohe, and Schweikardt showed that the query containment problem for monadic datalog on finite unranked labeled trees is \textit{Exptime}-complete when (a) considering unordered trees using the \textit{child}-axis, and when (b) considering ordered trees using the axes \textit{firstchild}, \textit{nextsibling}, and \textit{child}. Furthermore, when allowing to use also the \textit{descendant}-axis, the query containment problem was shown to be solvable in 2-fold exponential time, but it remained open to determine the problem’s exact complexity in presence of the descendant-axis. The present paper closes this gap by showing that, in the presence of the descendant-axis, the problem is $2\text{Exptime}$-hard.

1 Introduction

The query containment problem (QCP) is a fundamental problem that has been studied for various query languages. Datalog is a standard tool for expressing queries with recursion. From Cosmadakis et al. \cite{Cosmadakis} and Benedikt et al. \cite{Benedikt} it is known that the QCP for \textit{monadic} datalog queries on the class of all finite relational structures is $2\text{Exptime}$-complete.

Restricting attention to finite unranked labeled trees, Gottlob and Koch \cite{Gottlob} showed that on \textit{ordered} trees the QCP for monadic datalog is \textit{Exptime}-hard and decidable, leaving open the question for a tight bound. This gap was closed by Frochaux, Grohe, and Schweikardt in \cite{Frochaux} by giving a matching \textit{Exptime} upper bound for the QCP for monadic datalog on ordered trees using the axes \textit{firstchild}, \textit{nextsibling}, and \textit{child}. Similar results were obtained in \cite{Frochaux} also for \textit{unordered} finite labeled trees: in this setting, the QCP is \textit{Exptime}-complete for monadic datalog queries on unordered trees using the \textit{child}-axis.

For the case where queries are allowed to also use the \textit{descendant}-axis, \cite{Frochaux} presented a 2-fold exponential time algorithm for the QCP for monadic datalog on (ordered or unordered) trees. Determining the problem’s exact complexity in the presence of the \textit{descendant}-axis, however, was left open.

The present paper closes this gap by proving a matching $2\text{Exptime}$ lower bound (both, for ordered and for unordered trees). This gives a conclusive answer to a question posed by Abiteboul et al. in \cite{Abiteboul}, asking for the complexity of the

* This article is the full version of \cite{Frochaux}. 
QCP on unordered trees in the presence of the descendant-axis. Our 2Exptime-hardness proof for ordered trees is by a reduction from a 2Exptime-hardness result of [3] for the validity of conjunctive queries w.r.t. schema constraints. For obtaining the 2Exptime-hardness on unordered trees, we follow the approach of [3] and construct a reduction from the 2Exptime-complete word problem for exponential-space bounded alternating Turing machines [4].

The remainder of the paper is organised as follows. Section 2 fixes the basic notation. Section 3 presents a 2Exptime lower bound for the QCP on ordered trees using the axes firstchild, nextsibling, root, leaf, lastsibling, child, descendant. Section 4 is devoted to the 2Exptime lower bound for the QCP on unordered trees using only the axes child and descendant. We conclude in Section 5.

Proof details can be found in the appendix.

2 Trees and Monadic Datalog (mDatalog)

Throughout this paper, Σ will always denote a finite non-empty alphabet. By \(\mathbb{N}\) we denote the set of non-negative integers, and we let \(\mathbb{N}_{>1} := \mathbb{N} \setminus \{0\}\).

**Relational Structures.** As usual, a schema \(\tau\) consists of a finite number of relation symbols \(R\), each of a fixed arity \(ar(R) \in \mathbb{N}_{>1}\). A \(\tau\)-structure \(A\) consists of a finite non-empty set \(A\) called the domain of \(A\), and a relation \(R^A \subseteq A^{ar(R)}\) for each relation symbol \(R \in \tau\). It will often be convenient to identify \(A\) with the set of atomic facts of \(A\), i.e., the set \(\text{atoms}(A)\) consisting of all facts \(R(a_1, \ldots, a_{ar(R)})\) for all relation symbols \(R \in \tau\) and all tuples \((a_1, \ldots, a_{ar(R)}) \in R^A\).

If \(\tau\) is a schema and \(\ell\) is a list of relation symbols, we write \(\tau^\ell\) to denote the extension of the schema \(\tau\) by the symbols in \(\ell\). Furthermore, \(\tau_\Sigma\) denotes the extension of \(\tau\) by new unary relation symbols \(\text{label}_\alpha\), for all \(\alpha \in \Sigma\).

**Unordered Trees.** An unordered \(\Sigma\)-labeled tree \(T = (V^T, \lambda^T, E^T)\) consists of a finite non-empty set \(V^T\) of nodes, a function \(\lambda^T: V^T \to \Sigma\) assigning to each node \(v\) of \(T\) a label \(\lambda(v) \in \Sigma\), and a set \(E^T \subseteq V^T \times V^T\) of directed edges such that the directed graph \((V^T, E^T)\) is a rooted tree where edges are directed from the root towards the leaves. We represent such a tree \(T\) as a relational structure of domain \(V^T\) with unary and binary relations: For each label \(\alpha \in \Sigma\), \(\text{label}_\alpha(x)\) expresses that \(x\) is a node with label \(\alpha\); \(\text{child}(x, y)\) expresses that \(y\) is a child of node \(x\); \(\text{root}(x)\) expresses that \(x\) is the tree’s root node; \(\text{leaf}(x)\) expresses that \(x\) is a leaf; and \(\text{desc}(x, y)\) expresses that \(y\) is a descendant of \(x\) (i.e., \(y\) is a child or a grandchild or . . . of \(x\)). We denote this relational structure representing \(T\) by \(S_u(T)\), but when no confusion arises we simply write \(T\) instead of \(S_u(T)\).

The queries we consider for unordered trees are allowed to make use of at least the predicates \(\text{label}_\alpha\) and \(\text{child}\). We fix the schema \(\tau_u := \{\text{child}\}\).

**Ordered Trees.** An ordered \(\Sigma\)-labeled tree \(T = (V^T, \lambda^T, E^T, \text{order}^T)\) has the same components as an unordered \(\Sigma\)-labeled tree and, in addition, \(\text{order}^T\) fixes for each node \(u\) of \(T\) a strict linear order of all the children of \(u\) in \(T\).

To represent such a tree as a relational structure, we use the same domain and the same predicates as for unordered \(\Sigma\)-labeled trees, along with three further
predicates $\text{fc}$ (“first-child”), $\text{ns}$ (“next-sibling”), and $\text{ls}$ (“last sibling”), where $\text{fc}(x, y)$ expresses that $y$ is the first child of node $x$ (w.r.t. the linear order of the children of $x$ induced by $\text{order}^T$); $\text{ns}(x, y)$ expresses that $y$ is the right sibling of $x$ (i.e., $x$ and $y$ have the same parent $p$, and $y$ is the immediate successor of $x$ in the linear order of $p$’s children given by $\text{order}^T$); and $\text{ls}(x)$ expresses that $x$ is the rightmost sibling (w.r.t. the linear order of the children of $x$’s parent given by $\text{order}^T$). We denote this relational structure representing $T$ by $S_o(T)$, but when no confusion arises we simply write $T$ instead of $S_o(T)$.

The queries we consider for ordered trees are allowed to make use of at least the predicates $\text{label}_o$, $\text{fc}$, and $\text{ns}$. We fix the schemas $\tau_o := \{ \text{fc}, \text{ns} \}$ and $\tau_{\text{GK}} := \tau_o^{\text{root}, \text{leaf}, \text{ls}}$. In [11], Gottlob and Koch used $\tau_{\text{GK}, \Sigma}$-structures to represent ordered $\Sigma$-labeled trees.

**Datalog.** We assume that the reader is familiar with the syntax and semantics of datalog (cf., e.g., [6][11]). Predicates that occur in the head of some rule of a datalog program $\mathcal{P}$ are called intensional, whereas predicates that only occur in the body of rules of $\mathcal{P}$ are called extensional. By $\text{idb}(\mathcal{P})$ and $\text{edb}(\mathcal{P})$ we denote the sets of intensional and extensional predicates of $\mathcal{P}$, resp. We say that $\mathcal{P}$ is of schema $\tau$ if $\text{edb}(\mathcal{P}) \subseteq \tau$. We write $\mathcal{T}_\mathcal{P}$ to denote the immediate consequence operator associated with a datalog program $\mathcal{P}$. Recall that $\mathcal{T}_\mathcal{P}$ maps a set $C$ of atomic facts to the set of all atomic facts that are derivable from $C$ by at most one application of the rules of $\mathcal{P}$. The monotonicity of $\mathcal{T}_\mathcal{P}$ implies that for each finite set $C$, the iterated application of $\mathcal{T}_\mathcal{P}$ to $C$ leads to a fixed point, denoted by $\mathcal{T}_\mathcal{P}^\omega(C)$, which is reached after a finite number of iterations.

**Monadic datalog queries.** A datalog program belongs to monadic datalog (mDatalog, for short), if all its intensional predicates have arity 1.

A unary monadic datalog query of schema $\tau$ is a tuple $Q = (\mathcal{P}, P)$ where $\mathcal{P}$ is a monadic datalog program of schema $\tau$ and $P$ is an intensional predicate of $\mathcal{P}$. $\mathcal{P}$ and $P$ are called the program and the query predicate of $Q$. When evaluated in a finite $\tau$-structure $\mathcal{A}$ that represents a labeled tree $T$, the query $Q$ results in the unary relation $Q(T) := \{ a \in A : P(a) \in T_\mathcal{P}(\text{atoms}(\mathcal{A})) \}$.

The Boolean monadic datalog query $Q_{\text{root}}$ specified by $Q = (\mathcal{P}, P)$ is the Boolean query with $Q_{\text{root}}(T) = \text{yes}$ iff the tree’s root node belongs to $Q(T)$.

The size $|Q|$ of a monadic datalog query $Q$ is the length of $Q = (\mathcal{P}, P)$ viewed as a string over a suitable alphabet.

**Expressive power of monadic datalog on trees.** On ordered $\Sigma$-labeled trees represented as $\tau_{\text{GK}, \Sigma}$-structures, monadic datalog can express exactly the same unary queries as monadic second-order logic [11] — for short, we will say “mDatalog(\tau_{\text{GK}}) = \text{MSO}(\tau_{\text{GK}})$ on ordered trees”. Since the $\text{child}$ and $\text{desc}$ relations are definable in $\text{MSO}(\tau_{\text{GK}})$, $\text{mDatalog}(\tau_{\text{GK}}) = \text{mDatalog}(\tau_{\text{GK}}^{\text{child}, \text{desc}})$ on ordered trees. Moreover, for (ordered or unordered) trees, every monadic Datalog query that uses the $\text{desc}$-axis can be rewritten in 1-fold exponential time into an equivalent monadic datalog query which uses the $\text{child}$-axis, but not the $\text{desc}$-axis (see the proof of Lemma 23 in the full version of [8]).

Using the monotonicity of the immediate consequence operator, one obtains that removing any of the predicates $\text{root}, \text{leaf}, \text{ls}$ from $\tau_{\text{GK}}$ strictly decreases the
expressive power of mDatalog on ordered trees (see [9]). By a similar reasoning one also obtains that on unordered trees, represented as \( \tau_{u,\Sigma}^{\text{root},\text{leaf},\text{desc}} \)-structures, monadic datalog is strictly less expressive than monadic second-order logic, and omitting any of the predicates \text{root}, \text{leaf} \) further reduces the expressiveness of monadic datalog on unordered trees [9].

The Query Containment Problem (QCP). Let \( \tau_{\Sigma} \) be one of the schemas used for representing (ordered or unordered) \( \Sigma \)-labeled trees as relational structures. For two unary queries \( Q_1 \) and \( Q_2 \) of schema \( \tau_{\Sigma} \), we write \( Q_1 \subseteq Q_2 \) to indicate that for every \( \Sigma \)-labeled tree \( T \) we have \( Q_1(T) \subseteq Q_2(T) \). Similarly, if \( Q_1 \) and \( Q_2 \) are Boolean queries of schema \( \tau_{\Sigma} \), we write \( Q_1 \subseteq Q_2 \) to indicate that for every \( \Sigma \)-labeled tree \( T \), if \( Q_1(T) = \text{yes} \) then also \( Q_2(T) = \text{yes} \). We write \( Q_1 \nsubseteq Q_2 \) to indicate that \( Q_1 \nsubseteq Q_2 \) does not hold. For a schema \( \tau \), the query containment problem (QCP) for mDatalog(\( \tau \)) on finite labeled trees receives as input a finite alphabet \( \Sigma \) and two (unary or Boolean) mDatalog(\( \tau_{\Sigma} \))-queries \( Q_1 \) and \( Q_2 \), and the task is to decide whether \( Q_1 \subseteq Q_2 \). From [8] we know:

**Theorem 1 (Frochaux et al. [8])** The QCP for mDatalog(\( \tau_{u,\Sigma}^{\text{root},\text{leaf},\text{desc}} \)) on unordered trees and for mDatalog(\( \tau_{\text{GK}}^{\text{child},\text{desc}} \)) on ordered trees can be solved in 2-fold exponential time.

### 3 2Exptime-hardness on Ordered Trees

**Theorem 2** The QCP for Boolean mDatalog(\( \tau_{\text{GK}}^{\text{child},\text{desc}} \)) on finite labeled ordered trees is 2Exptime-hard.

The proof is by a reduction based on a 2Exptime-hardness result of Björklund, Martens, and Schwentick [3]. For stating their result, we recall some notation used in [3]. A nondeterministic (unranked) tree automaton (NTA) \( A = (\Sigma, S, \Delta, F) \) consists of an input alphabet \( \Sigma \), a finite set \( S \) of states, a set \( F \subseteq S \) of accepting states, and a finite set \( \Delta \) of transition rules of the form \((s, \alpha) \rightarrow L\), where \( s \in S \), \( \alpha \in \Sigma \), and \( L \) is a regular string-language over \( S \). A run of the NTA \( A \) on an ordered \( \Sigma \)-labeled tree \( T \) is a mapping \( \rho : V_T \rightarrow S \) such that the following is true for all nodes \( v \) of \( T \), where \( \alpha \) denotes the label of \( v \) in \( T \): if \( v \) has \( n \geq 0 \) children \( u_1, \ldots, u_n \) (in order from the left to the right), then there exists a rule \((s, \alpha) \rightarrow L \) in \( \Delta \) such that \( \rho(v) = s \) and \( w_v \in L \), for the string \( w_v := \rho(u_1) \cdots \rho(u_n) \). In particular, if \( v \) is a leaf, then there must be a rule \((s, \alpha) \rightarrow L \) in \( \Delta \) such that \( \rho(v) = s \) and \( \varepsilon \in L \), where \( \varepsilon \) denotes the empty string.

A run \( \rho \) of \( A \) on \( T \) is accepting, if \( T \)'s root note \( v \) is labeled with an accepting state of \( A \), i.e., \( \rho(v) \in F \). A finite ordered \( \Sigma \)-labeled tree \( T \) is accepted by \( A \), if there exists an accepting run of \( A \) on \( T \). We write \( L(A) \) to denote the language of \( A \), i.e., the set of all finite ordered \( \Sigma \)-labeled trees that are accepted by \( A \).

To present an NTA \( A = (\Sigma, S, \Delta, F) \) as an input for an algorithm, the string-languages \( L \) that occur in the right-hand side of rules in \( \Delta \) are specified by NFAs \( A_L = (\Sigma_L, Q_L, \delta_L, q_L, F_L) \), whose input alphabet is \( \Sigma_L := S \), and where \( L \) is a finite set of states, \( \delta_L \subseteq (Q_L \times \Sigma_L \times Q_L) \) is a transition relation, \( q_L \in Q_L \) is the
initial state, and \( F_L \subseteq Q_L \) is the set of accepting states of \( A_L \). The size of \( A_L \) is \( |A_L| := |Q_L| + |\delta_L| \), and the size of \( A \) is the sum of \( |\Sigma|, |S|, |\Delta| \), and \(|A_L|\), for all \( L \in \text{str}(A) \), where \( \text{str}(A) \) is the set of all string-languages \( L \) that occur in the right-hand side of a rule in \( \Delta \).

In [3], NTAs are used to describe schema information. A Boolean query \( Q \) is said to be valid with respect to an NTA \( A \) if \( Q(T) = \text{yes} \) for every ordered \( \Sigma \)-labeled tree \( T \in L(A) \). The particular queries of interest here are Boolean \( CQ(\text{child, desc}) \) queries, i.e., Boolean conjunctive queries of schema \( \tau_{u, \Sigma}^{\text{desc}} = \{ \text{child, desc} \} \cup \{ \text{label}_\alpha : \alpha \in \Sigma \} \), for a suitable alphabet \( \Sigma \). The problem “validity of Boolean \( CQ(\text{child, desc}) \) w.r.t. a tree automaton” receives as input a Boolean \( CQ(\text{child, desc}) \) query \( Q \) and an NTA \( A \), and the task is to decide whether \( Q \) is valid with respect to \( A \).

**Theorem 3 (Björklund et al. [3])** Validity of Boolean \( CQ(\text{child, desc}) \) w.r.t. a tree automaton is 2EXPTIME-complete.

Our proof of Theorem 3 is via a polynomial-time reduction from the problem validity of Boolean \( CQ(\text{child, desc}) \) w.r.t. a tree automaton to the QCP for Boolean mDatalog(\( \tau_{u, \Sigma}^{\text{child, desc}} \)) on finite labeled ordered trees.

Let \( Q_{CQ} \) be a Boolean \( CQ(\text{child, desc}) \)-query, and let \( A \) be an NTA with input alphabet \( \Sigma \). We translate \( Q_{CQ} \) into an equivalent mDatalog(\( \tau_{u, \Sigma}^{\text{desc}} \))-query \( Q'_{CQ} = (P, P) \): If \( Q_{CQ} \) is of the form \( \text{Ans}() \leftarrow R_1(u_1), \ldots , R_\ell(u_\ell) \) for relational atoms \( R_1(u_1), \ldots , R_\ell(u_\ell) \), we choose an arbitrary variable \( x \) that occurs in at least one of these atoms, we use a new unary idb-predicate \( P \), and we let \( P \) be the program consisting of the two rules \( P(x) \leftarrow R_1(u_1), \ldots , R_\ell(u_\ell) \) and \( P(x) \leftarrow \text{child}(x,y), P(y) \).

Then, for every ordered \( \Sigma \)-labeled tree \( T \) we have \( Q'_{CQ, \text{Boo}l}(T) = \text{yes} \) if and only if \( Q_{CQ}(T) = \text{yes} \). The following Lemma 4 constructs, in time polynomial in the size of \( A \), an mDatalog(\( \tau_{u, \Sigma}^{\text{child, desc}} \))-query \( Q_A \) which is equivalent to \( A \), i.e., for every ordered \( \Sigma \)-labeled tree \( T \) we have \( Q_{A, \text{Boo}l}(T) = \text{yes} \) iff \( T \in L(A) \).

Note that \( Q_{CQ} \) is valid w.r.t. \( A \) if and only if \( Q_{A, \text{Boo}l} \subseteq Q'_{CQ, \text{Boo}l} \). Thus, we obtain the desired polynomial-time reduction, showing that the QCP for Boolean mDatalog(\( \tau_{u, \Sigma}^{\text{child, desc}} \)) on finite ordered \( \Sigma \)-labeled trees inherits the 2EXPTIME-hardness from the problem “validity of Boolean \( CQ(\text{child, desc}) \) w.r.t. a tree automaton”. All that remains to finish the proof of Theorem 2 is to prove the following Lemma 4.

**Lemma 4** For every NTA \( A = (\Sigma, S, \Delta, F) \) there is an mDatalog(\( \tau_{u, \Sigma}^{\text{child, desc}} \))-query \( Q = (P, P) \), such that for every finite ordered \( \Sigma \)-labeled tree \( T \) we have \( Q_{\text{Boo}l}(T) = \text{yes} \) iff \( T \in L(A) \). Furthermore, \( Q \) is constructible from \( A \) in time polynomial in the size of \( A \).

**Proof.** We construct a monadic datalog program \( P \) which, for every node \( v \) of \( T \), computes information on all states that \( A \) can assume at node \( v \), i.e., all states \( s \in S \) for which there is a run \( \rho \) of \( A \) on the subtree of \( T \) rooted at \( v \), such that \( \rho(v) = s \). To this end, for every state \( s \in S \), we will use an idb-predicate \( s \).
The query $Q_{\text{Root}}$ will accept an input tree $T$ if there is an accepting state $s \in F$ such that $s(\text{root}^T) \in \mathcal{T}^\mathcal{P}(T)$, where \text{root}^T denotes the root of $T$. The program $\mathcal{P}$ is constructed in such a way that it performs a generalised version of the well-known powerset construction.

Recall that the transition rules of $\mathcal{A}$ are of the form $(s, \alpha) \rightarrow L$, where $s \in S$, $\alpha \in \Sigma$, and $L$ is a regular string-language over $S$, specified by an NFA $\mathcal{A}_L = (\Sigma_L, Q_L, \delta_L, q_L, F_L)$ with $\Sigma_L = S$ and $\delta_L \subseteq (Q_L \times \Sigma_L \times Q_L)$. W.l.o.g., we assume that the state sets of all the NFAs are mutually disjoint, and disjoint with $S$.

To emulate the standard powerset construction of the NFA $\mathcal{A}_L$, we use an idb-predicate $q$ for every state $q \in Q_L$, and an extra idb-predicate $\text{Acc}_L$. If $u_1, \ldots, u_n$ are the children of a node $v$ in an input tree $T$, the NFA $\mathcal{A}_L$ processes the strings over alphabet $S$ that are of the form $s_1 \cdots s_n$, where $s_i$ is a state that $\mathcal{A}$ can assume at node $u_i$ (for every $i \in \{1, \ldots, n\}$). We start by letting $\mathcal{P}_L := \emptyset$ and then add to $\mathcal{P}_L$ the following rules: For the initial state $q_L$ of $\mathcal{A}_L$, consider all $s \in S$ and $q \in Q_L$ such that $(q_L, s, q) \in \delta_L$, and add to $\mathcal{P}_L$ the rule

$$q(x) \leftarrow \text{fc}(y, x), \ s(x).$$

Afterwards, for every transition $(q, s, q') \in \delta_L$, add to $\mathcal{P}_L$ the rule

$$q'(x') \leftarrow q(x), \ \text{ns}(x, x'), \ s(x').$$

Finally, for every accepting state $q \in F_L$ of $\mathcal{A}_L$, add to $\mathcal{P}_L$ the rule

$$\text{Acc}_L(x) \leftarrow \text{ls}(x), \ q(x).$$

Clearly, the program $\mathcal{P}_L$ can be constructed in time polynomial in $|\mathcal{A}_L|$.

Now, we are ready to construct the monadic datalog program $\mathcal{P}$ that simulates the NTA $\mathcal{A}$. We start by letting $\mathcal{P}$ be the disjoint union of the programs $\mathcal{P}_L$, for all $L \in \text{strL}(\mathcal{A})$. The computation of $\mathcal{A}$ on an input tree $T$ starts in the leaves of $T$. Thus, to initiate the simulation of $\mathcal{A}$, we consider every rule $(s, \alpha) \rightarrow L$ in $\Delta$, where $\varepsilon \in L$. For each such rule, we add to $\mathcal{P}$ the rule

$$s(x) \leftarrow \text{label}_s(x), \ \text{leaf}(x).$$

Note that for each $L \in \text{strL}(\mathcal{A})$, the program $\mathcal{P}_L$ ensures that every last sibling $u_n$ of a node $v$ will be marked by $\text{Acc}_L(u_n)$ iff the states of $\mathcal{A}$ assigned to $u_n$ and its siblings form a string in $L$. To transfer this information from the last sibling to its parent node, we add to $\mathcal{P}$ the rule

$$\text{child}_{\text{Acc}_L}(y) \leftarrow \text{child}(y, x), \ \text{ls}(x), \ \text{Acc}_L(x),$$

where $\text{child}_{\text{Acc}_L}$ is a new idb-predicate, for every $L \in \text{strL}(\mathcal{A})$. Afterwards, we consider every rule $(s, \alpha) \rightarrow L$ in $\Delta$, and add to $\mathcal{P}$ the rule

$$s(x) \leftarrow \text{child}_{\text{Acc}_L}(x), \ \text{label}_s(x).$$

Finally, to test if $\mathcal{A}$ accepts an input tree $T$, we add rules to test whether $T$’s root is assigned an accepting state of $\mathcal{A}$. To this end, we consider every accepting state $s \in F$ of $\mathcal{A}$ and add to $\mathcal{P}$ the rule

$$P(x) \leftarrow \text{root}(x), \ s(x).$$

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1 Note that “$\varepsilon \in L$?” can be checked by simply checking whether $q_L \in F_L$. 


This finishes the construction of the program $P$ and the query $Q = (P, P)$. Clearly, $P$ is a monadic datalog program of schema $\tau_{\text{child}}^G \Sigma$, and $Q$ can be constructed in time polynomial in $|A|$. It is not difficult, but somewhat tedious, to verify that, as intended by the construction, indeed for every finite ordered $\Sigma$-labeled tree $T$ we have $Q_{\text{Bool}}(T) = \text{yes}$ if, and only if, there exists an accepting run of the NTA $A$ on $T$. This completes the proof of Lemma 4. ⊓ ⊔

4 2Exptime-hardness on Unordered Trees

Our next aim is to transfer the statement of Theorem 2 to unordered trees. Precisely, we will show the following.

Theorem 5 The QCP for Boolean mDatalog($\tau_{\text{desc}}^u$) on finite labeled unordered trees is 2Exptime-hard.

For proving Theorem 5 we cannot directly build on Björklund et al.’s Theorem 3 since their NTAs explicitly refer to ordered trees.

By constructing suitable reductions, we can show that proving Theorem 5 boils down to proving the following Theorem 6, which deals with the emptiness problem on trees over a ranked alphabet.

For the remainder of this section, $\Sigma'$ will denote a ranked finite alphabet, i.e., $\Sigma'$ is a finite set of symbols, and each symbol $\alpha \in \Sigma'$ is equipped with a fixed arity $ar(\alpha) \in \mathbb{N}$. An unordered ranked $\Sigma'$-labeled tree is an unordered $\Sigma'$-labeled tree where each node labeled with symbol $\alpha \in \Sigma'$ has exactly $ar(\alpha)$ children. For a Boolean mDatalog($\tau_{\text{desc}}^u, \Sigma'$)-query $Q$, we say that $Q$ is unsatisfiable by unordered ranked trees (in symbols: $Q = \emptyset$) if for every finite unordered ranked $\Sigma'$-labeled tree $T$ we have $Q(T) = \emptyset$. The emptiness problem for Boolean mDatalog($\tau_{\text{desc}}^u, \Sigma'$) on finite unordered ranked $\Sigma'$-labeled trees receives as input a Boolean mDatalog($\tau_{\text{desc}}^u, \Sigma'$)-query $Q$, and the task is to decide whether $Q = \emptyset$.

The main technical step needed for proving Theorem 5 is to prove the following.

Theorem 6 There is a ranked finite alphabet $\Sigma'$, such that the emptiness problem for Boolean mDatalog($\tau_{\text{desc}}^u, \Sigma'$) on finite unordered ranked $\Sigma'$-labeled trees is 2Exptime-hard.

For the proof of Theorem 6 we can build on the approach used by Björklund et al. for proving Theorem 3. As in [3], we proceed by a reduction from the word problem for exponential-space bounded alternating Turing machines, which is known to be 2Exptime-complete [4]. The remainder of this section is devoted to the proof of Theorem 6.

An alternating Turing machine (ATM) is a nondeterministic Turing machine $A = (Q, \Sigma, \Gamma, \delta, q_0)$ whose state space $Q$ is partitioned into universal states $Q_u$, existential states $Q_\exists$, an accepting state $q_a$, and a rejecting state $q_r$. The ATM’s tape cells are numbered $0, 1, 2, \ldots$. A configuration of $A$ is a finite string of the form $w_1q_2$ with $w_1, w_2 \in \Gamma^*$ and $q \in Q$, representing the situation where the ATM’s tape contains the word $w_1w_2$, followed by blanks, the ATM’s current state
is \( q \), and the head is positioned at the first letter of \( w_2 \). A configuration \( w_1qw_2 \) is a halting (universal, existential, resp.) configuration if \( q \in \{ q_a, q_r \} \) (\( q \in Q_f \), \( q \in Q_\exists \), resp.). W.l.o.g., no halting configuration has a successor configuration, and every halting configuration is of the form \( qw \). A computation tree \( T_k \) of the ATM \( A \) on input \( w \in \Sigma^* \) is a tree labeled with configurations of \( A \), such that the root of \( T_k \) is labeled by \( q_0w \), and for each node \( v \) of \( T_k \) labeled by \( w_1qw_2 \),

\[ - \text{if } q \in Q_\exists, \text{ then } u \text{ has exactly one child, and this child is labeled with a successor configuration of } w_1qw_2, \]

\[ - \text{if } q \in Q_f, \text{ then } u \text{ has a child } v \text{ for every successor configuration } w_1'q'w_2', \text{ and } \]

\[ v \text{ is labeled by } w_1'q'w_2', \]

\[ - \text{if } q \in \{ q_a, q_r \}, \text{ then } u \text{ is a leaf of } T_k. \]

A computation tree is accepting if all its branches are finite and all its leaves are labeled by configurations with state \( q_a \). The language \( L(A) \) of \( A \) is defined as the set of all words \( w \in \Sigma^* \), for which there exists an accepting computation tree of \( A \) on \( w \). W.l.o.g., we will assume that the ATM is normalized, i.e., every non-halting configuration has precisely two successor configurations, each universal step only affects the state of the machine, and the machine always alternates between universal and existential states.

The proof of Theorem \([3]\) proceeds by a reduction from the word problem for exponential-space bounded ATMs \( A \). The reduction itself will be done from an ATM with empty input word. To this end, we construct, in the canonical way, for the given exponential-space bounded ATM \( A \) and the given word \( w \in \Sigma^* \) an ATM \( A_w \) that works in space exponential in the size of \( w \) and accepts the empty word if, and only if, \( A \) accepts \( w \). Since \( A \) is exponential-space bounded, the non-blank portion of the ATM’s tape during a computation of \( A_w \) will never be longer than \( 2^n \), where \( n \) is polynomial in the size \( |w| \) of the original input.

The crucial point of the reduction is to find an encoding of computation trees of \( A_w \) on empty input, which can be verified by a mDatalog(\( ^{desc}_n \Sigma \))-query that can be constructed in time polynomial in the size of \( A_w \). For this, it is necessary to find a smart encoding of the tape inscription of length \( 2^n \). This encoding shall allow to compare the content of every tape cell with the same tape cell of the successor configuration. To achieve this, we adapt the encoding of Björklund et al. \([3]\); in particular, we use their very elegant “navigation gadgets”.

We choose a fixed ranked finite alphabet \( \Sigma' \) which, among other symbols, contains a 0-ary symbol \( \bot \), unary symbols \( r, p, m \), 0, 1, binary symbols CT\(^{left}_3 \), CT\(^{right}_3 \), and 3-ary symbols CT\(_f \) and \( s \). Consider a computation tree \( T_{A_w} \) of a normalized ATM \( A_w = (Q, \Sigma, \Gamma, \delta, q_0, \emptyset) \), see Figure \([1]\).

We fix an arbitrary order on the children of nodes in \( T_{A_w} \), such that every universal node has a left child and a right child. The encoding \( T := \text{enc}(T_{A_w}) \) is the ranked \( \Sigma' \)-labeled unordered tree obtained from \( T_{A_w} \) by replacing every node \( v \) labeled \( w_1qw_2 \) with a \( \Sigma' \)-labeled ranked tree \( \text{enc}(t_v) \), as follows:

\[ - \text{if } v \text{ is universal, then the root of } \text{enc}(t_v) \text{ is labeled with CT\(_f \)}, \]

\[ - \text{if } v \text{ is existential, and } v \text{ is the root of } T_{A_w} \text{ or } v \text{ is the left child of a universal node, then the root of } \text{enc}(t_v) \text{ is labeled with CT\(^{left}_3 \)}]. \]
Fig. 1. (a) A part of a computation tree \(T_{A_w}\) where the node \(v_1\) labeled by \(w'_1q_1w''_1\) is universal, and its children are existential. The node \(v_2\) labeled by \(w'_2q_2w''_2\) is the right child of \(v_1\). The node \(v_3\) has one child, the univeral node \(v_5\). (b) The replacement of \(v_1\) is a tree with a root node labeled by \(CT\) and with three children, the first is labeled by \(r\) and is the root of the subtree encoding the configuration in \(v_1\), the second is the replacement for its left child, and the third is the replacement for its right child. The obtained tree \(T := \text{enc}(T_{A_w})\) is an unordered ranked \(\Sigma'\)-labeled tree.

- if \(v\) is existential, and \(v\) is the right child of a universal node, then the root of \(\text{enc}(t_v)\) is labeled with \(CT_{\exists}^{\text{right}}\),
- exactly one child of the root of \(\text{enc}(t_v)\) is labeled by \(r\) (this will be the root of the subtree that encodes the configuration at \(v\)), and
- for each child \(u\) of \(v\) in \(T_{A_w}\), \(\text{enc}(t_v)\) has a subtree \(\text{enc}(t_u)\), which is the encoded subtree of \(T_{A_w}\) obtained by the replacement of \(u\).

The subtree \(\gamma_r\) rooted at the \(r\)-labeled child of the root of \(\text{enc}(t_v)\), encodes the configuration \(c := w_1qw_2\) represented by node \(v\) in \(T_{A_w}\). Since \(A\) is exponential-space bounded, the tape inscription of \(c\) has length \(< 2^n\). For representing \(c\), we use a full binary ordered tree of height \(n\). The path from the root to a leaf specifies the address of the tape cell represented by the leaf, and the leaf carries information on the tape cell’s inscription and, in case that the tape cell is the current head position, also information on the current state; all this information is encoded by a suitable tape cell gadget that is attached to the “leaf”. The number \(k\) of possible tape cell inscriptions (enriched with information on the current state) is polynomial in \(|A_w|\). The nodes of the “full binary tree” are called skeleton nodes and are labeled \(s\). To ensure that the desired query \(Q\) can be constructed in polynomial time, we attach to each skeleton node a navigation gadget \([3]\), which is a path of length 4. To indicate that a node is a left (resp., right) child, this gadget is labeled \(p-0-1-\perp\) (resp., \(p-1-0-\perp\)). See Figure 2 for an illustration of the navigation gadget and the tape cell gadget.

Given an ATM \(A\) and a word \(w \in \Sigma^*\), we construct in polynomial time an mDatalog\((\tau_{\text{desc}}, A')\)-query \(Q = (P, \text{Ans})\) such that \(Q_{\text{Bool}} \neq \emptyset\) iff there is an accepting computation tree for \(A_w\) on \(\varepsilon\), i.e., \(w \in L(A)\). The query \(Q\) consists of two parts, one to verify that the structure of the input tree represents an encoded computation tree, and the other to verify consistency with the ATM’s transition relation. Details can be found in the appendix. The particular choice
Fig. 2. (a) A skeleton node and its navigation gadget, indicating that the node is its parent’s left child. (b) A skeleton node encoding a leaf of the configuration tree. This leaf is its parent’s right child. It has a tape cell gadget \( m \) followed by \( k \) digits, the \( i \)-th of which is labeled with 1 iff the tape cell’s inscription is represented by the number \( i \).

of the navigation gadgets ensures that \( Q \) can be constructed in time polynomial in the size of \( A \) and \( w \). The only point where we make essential use of the \texttt{desc}-predicate is during the comparison of the cells by using the navigation gadgets.

5 Final Remarks

Along with the upper bound provided by Theorem 1 and since \( \tau_u^{\text{desc}} \subseteq \tau_o^{\text{child,desc}} \), Theorem 5 implies the following corollary, which summarizes our main results.

\textbf{Corollary 7} The QCP is \textsc{2Exptime}-complete for Boolean mDatalog(\( \tau_u^{\text{desc}} \)) on finite labeled unordered trees, and for Boolean mDatalog(\( \tau_o^{\text{child,desc}} \)) on finite labeled ordered trees.

By applying standard reductions, the \textsc{2Exptime}-completeness results of Corollary 4 carry over from the QCP to the equivalence problem. When restricting attention to ranked trees over a ranked finite alphabet, the \textsc{2Exptime}-completeness results also carry over to the emptiness problem. For unranked labeled trees, the emptiness problem for mDatalog(\( \tau_o^{\text{child,desc}} \)) is in \textsc{2Exptime}, but we currently do not have a matching \textsc{2Exptime}-hardness result.

An overview of the currently known results is given in Table 1 for further information and detailed proofs we refer to [7].
Table 1. Complexity of monadic datalog on finite labeled trees; $N \subseteq \{\text{root, leaf}\}$ and $M \subseteq \{\text{root, leaf, ls, child}\}$; “c” (“h”) means “complete” (“hard”).

|       | $\tau_N$ | $\tau_M$ | $\tau_{N \cup \{\text{desc}\}}$ | $\tau_{M \cup \{\text{child, desc}\}}$ | $\tau_{\text{child, desc}}$ |
|-------|-----------|-----------|-------------------------------|---------------------------------|-----------------|
| Emptiness | Exptime-c | Exptime-h & in 2Exptime | 2Exptime-c | Exptime-c | unranked rank ed |
| Equivalence | Exptime-c | 2Exptime-c | 2Exptime-c | unranked rank ed |
| Containment | Exptime-c | 2Exptime-c | 2Exptime-c | unranked rank ed |
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APPENDIX

A Hardness on Ranked Trees

Theorem 6 (restated) There is a ranked finite alphabet $\Sigma'$, such that the emptiness problem for Boolean mDatalog($\tau_{\text{desc}}$) on finite unordered ranked $\Sigma'$-labeled trees is $2\text{EXPTIME}$-hard.

The proof idea of Theorem 6 is based on the proof of the Theorem 3 presented in the full version of the MFCS publication by Björklund, Martens, and Schwentick. The used alternating Turing machine was introduced at FOCS’76 by Chandra and Stockmeyer, as well as by Kozen, and presented in a joint journal publication in 1981.[4]

An alternating Turing machine (ATM, for short) $A = (Q, \Sigma, \Gamma, \delta, q_0)$ consists of

- a finite set of states $Q$ partitioned into universal states $Q_\forall$, existential states $Q_\exists$, an accepting state $q_a$, and a rejecting state $q_r$. 

the finite input alphabet $\Sigma$,

- the finite tape alphabet $\Gamma \supset \Sigma$, that contains the special blank symbol $\blank$,

- the initial (or, starting) state $q_0$ and

- the transition relation $\delta \subseteq ((Q \times \Gamma) \times (Q \times \Gamma \times \{L, R, S\}))$).

As usual the letters $L$, $R$, and $S$ denote the directions left, right, and stay in which the head on the tape is moved.

A configuration $c$ of $A$ is given by specifying its state, the content of its tape together with the position of the tape head. Thus, we interpret a string of the form $w_1qw_2$ with $w_1, w_2 \in \Gamma^*$, $q \in Q$ as the configuration in which the tape contains the word $w_1w_2$, followed by blanks, the head’s tape position is the first letter of $w_2$, and $q$ is the current state of the machine. A transition rule $((q, a), (q', b, D)) \in \delta$ denotes a step of $A$ by reading in state $q$ the letter $a \in \Gamma$, overwriting $a$ on the current head position by $b \in \Gamma$, moving the head depending on $D \in \{L, R, S\}$ one position to the left, to right, or stay, and finally, switching to state $q'$. A configuration $c'$ obtained by applying a rule of $\delta$ to a given configuration $c$ is called successor configuration of $c$. The configuration $w_1bwqw_2$, for example, is a successor configuration of $w_1qw_2$ obtained by applying the transition rule $((q, a), (q', b, R))$. A configuration $w_1qw_2$ is a halting configuration if $q$ is either the accepting state $q_a$ or the rejecting state $q_r$. Without loss of generality, we can assume that there is no successor configuration of any halting configuration, and furthermore, before halting, the automaton moves its head to the left on the first non-blank symbol on the tape, so each halting configuration is of the form $qw$.

A computation tree $T_A$ of the ATM $A$ on input $w \in \Sigma^*$ is a tree labeled with configurations of $A$, such that the root of $T_A$ is labeled by $q_0w$, and for each node $u$ of $T_A$ labeled by $w_1qw_2$,

- if $q \in Q_3$, then $u$ has exactly one child, and this child is labeled with a successor configuration of $w_1qw_2$,

- if $q \in Q_2$, then $u$ has a child $v$ for every successor configuration $w_1q'w_2'$ of $w_1qw_2$, and $v$ is labeled by $w_1q'w_2'$,

- if $q \in \{q_a, q_r\}$, then $u$ is a leaf of $T_A$.

Observe, that $T_A$ can be infinite, since $A$ may have non-halting computation branches. A computation tree is accepting if all its branches are finite and all its leaves are labeled by configurations in state $q_a$. As usually, the language $L(A)$ of the ATM $A$ is the set of words $w \in \Sigma^*$ for which there exists an accepting computation tree of $A$ on $w$.

We say that an ATM is normalized if every non-halting configuration has precisely two successor configurations, each universal step only affects the state of the machine, and additionally, the machine always proceeds from an universal state to an existential state, and vice versa. It is easy to verify that for every alternating Turing machine $A$ there exists a normalized alternating Turing machine $\tilde{A}_n$ with $L(A) = L(\tilde{A}_n)$, and $\tilde{A}_n$ can be constructed from $A$ within polynomial time.

Now, we are ready to prove Theorem 6.
Proof of Theorem 6:

Our proof proceeds by a reduction from the word problem for exponential space bounded ATM $A$. In this problem, the input consists on an exponential space bounded ATM $A$, and an input word $w$ for $A$, and the task is to decide if $w \in L(A)$.

In [4] this problem was shown to be $2\text{Exptime}$-complete.

Our reduction will be done from an ATM with empty input. Therefore, we construct for the given ATM $A$ and the given word $w$ an ATM $A_w$ that works in space exponential in the size $w$ and accepts the empty input word if and only if $A$ accepts $w$. To do this, we let $A_w$ start by writing $w$ on the empty tape, afterwards $A_w$ returns to the leftmost tape position and finally, it starts to simulate the original machine $A$. W.l.o.g., we can assume that $A_w$ is normalized and since the computation is exponentially space bounded, the non-blank portion of the tape during the computation of $A_w$ is never longer that $2^n$, where $n$ is polynomial in the size $|w|$ of the original input word.

We will choose a suitable ranked alphabet $\Sigma'$, independent from $A_w$. Within polynomial time, we construct an mDatalog($\tau_{\text{desc}}^{u,\Sigma'}$)-query $Q = (P, \text{Ans})$ such that

$$Q \neq \emptyset \iff \text{there is an accepting computation tree for } A_w \iff w \in L(A).$$

Since $2\text{Exptime}$ is closed under complement, it implies that the emptiness problem for Boolean mDatalog($\tau_{\text{desc}}^{u,\Sigma'}$) on ranked unordered labeled trees is hard for $2\text{Exptime}$.

In the next paragraphs, we present the encoding of the computation tree that is basically taken from [3] and includes the encoding of the configuration tree, both are adapted to our problem. So, let $T_{k_w}$ be a computation tree of $A_w = (Q, \Sigma, \Gamma, \delta, q_0)$ (cf. Figure 1), we fix some arbitrary order of the children of each universal node such that every universal node has a left and a right child. Now the encoding $T := \text{enc}(T_{k_w})$ can be obtained from $T_{k_w}$ by replacing every node $v$ labeled by $w_1qw_2$ with a tree $\text{enc}(t_v)$, as follows:

- if $v$ is universal, then the root of $\text{enc}(t_v)$ is labeled with $\text{CT}_v$,
- if $v$ is existential, and $v$ is the root of $T_{k_w}$ or $v$ is the left child of a universal node, then the root of $\text{enc}(t_v)$ is labeled with $\text{CT}_{\text{left}}^v$,
- if $v$ is existential, and $v$ is the right child of a universal node, then the root of $\text{enc}(t_v)$ is labeled with $\text{CT}_{\text{right}}^v$,
- exactly one child of the root of $\text{enc}(t_v)$ is labeled by $r$ (this will be the root of the subtree that encodes the configuration at $v$), and
- for each child $u_i$ of $v$ in $T_{k_w}$, $\text{enc}(t_v)$ has a subtree $\text{enc}(t_{u_i})$, which is the encoded subtree of $T_{k_w}$ obtained by the replacement of $u_i$.

The set of subtrees denoted by their root label $r$ encode the configurations that is originally labeled the computation tree. We have to navigate through $2^n$ tape

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2 A node $u$ is an universal node if it is labeled by a configuration $w_1qw_2$ where $q$ is an universal state. If $q$ is an existential state then $u$ is existential.

3 In fact, for a non halting configuration there is exactly one child if $v$ is existential or otherwise, if $v$ is universal, there are exactly two children since $A_w$ is normalized.
cells and we must be able to compare the \( i \)-th cell of one configuration with the \( i \)-th cell of the predecessor configuration. Thus, the configuration tree is basically a binary tree of height \( n \) that has \( 2^n \) leaves to carry the information for the tape cells, together with the information of the current state of the machine and the position of the head. This sequence of \( 2^n \) configuration cells will carry the whole information about the configuration of the machine in this working step. To this end, the set of configuration cells is partitioned into three types.

- The set \( \text{BCells} \) of basic cells is equal to \( \Gamma \). A basic cell represents a tape cell that is not currently visited by the head and also is not visited in the predecessor configuration.
- The set \( \text{CCells} \) of current tape head cells is equal to \( \Gamma \times \delta \). The letter from \( \Gamma \) represents the tape content in the actual position that is currently visited by the head, while the transition from \( \delta \) is the transition which leads to the actual configuration.
- The set \( \text{PCells} \) of previous tape head cells is equal to \( \Gamma \times (Q \times \Gamma) \) and represent tape cells that were visited by the head in the predecessor configuration, but not in the current one. The first letter from \( \Gamma \) represents the actual content on the tape in this cell and the pair \( (Q \times \Gamma) \) the previous state and tape content in the predecessor configuration.

Observe, the number \( k \) of all possible configuration cells for \( A_w \) is polynomial in the size of the automaton and so we can refer to each possible configuration cell a natural number \( i \) in \( \{1, \ldots, k\} \).

Now, it is necessary to fix a set of constraints, that allows to decide whenever a sequence \( C_1 \) of \( 2^n \) configuration cells is a valid successor configuration of another sequence \( C_0 \). We start with constraints to ensure a degree of consistency inside a given sequence. The set \( H(A_w) \) of horizontal constraints consists of the following rules:

(H1) The only cell allowed to the left of a cell \( (a, ((q_1, b), (q_2, c, R))) \in \text{CCells} \) is the cell \( (c, (q_1, b)) \in \text{PCells} \).
(H2) The only cell allowed to the right of a cell \( (a, ((q_1, b), (q_2, c, L))) \in \text{CCells} \) is the cell \( (c, (q_1, b)) \in \text{PCells} \).
(H3) The only cell allowed to the right of the basic cell \( \omega \in \Gamma \) is \( \omega \) itself.

To fix the set \( V(A_w) \) of vertical constraints between two consecutive sequences \( C_0 \) and \( C_1 \), we imagine the predecessor is lying cell by cell on top of its successor such that the \( i \)-th configuration cell of \( C_0 \) is lying on top of the \( i \)-th cell of \( C_1 \).

(V1) If the \( i \)-th cell is a BCell \( a \in \Gamma \) then the only allowed cells on the \( i \)-th tape position in a successor configuration are \( a \) itself and any CCell \( (a, ((q_1, b), (q_2, c, m))) \) where \( m \in \{L, R\} \). The latter is the case that the automaton \( A_w \) just moved to this cell, coming from the left or the right. The letter on this position is currently untouched, but the letter in the left (right) neighbor is overwritten if \( b \neq c \) and \( m = L \ (m = R) \).

(V2) If the \( i \)-th cell is a CCell \( (a, ((q_1, b), (q_2, c, m))) \) then the only allowed cells on the \( i \)-th tape position in a successor configuration are any \( (d, (q_2, a)) \in \text{PCells} \) and any \( (d, ((q_2, a), (q_3, d, m'))) \in \text{CCells} \) where \( m' = S \).
If the \(i\)-th cell is a PCell \((a, (q, b))\) then the only allowed cells on the \(i\)-th tape position in a successor configuration are the BCell \(a\) and any CCell \((a, ((q_1, b), (q_2, c, m)))\) where \(m \in \{L, R\}\).

Figure 3 illustrates an example of valid transitions respecting this constraints. It is easy to verify that if \(C_0\) is a valid encoding of a configuration, \(C_1\) is a valid encoding of a successor configuration if and only if all horizontal and vertical conditions are satisfied.

| \(C_s\)         | BCell | CCell          | PCell          |
|-----------------|-------|----------------|----------------|
| \(\cdots\)     | \(e\) | \(b\) \((q, c)\), \((q', f, L)\) | \(f\) \((q, c)\) |
| \(\cdots\)     |       |                |                |

\(C_{s+1}\)

| \(\cdots\) | BCell | CCell          | BCell          |
|-------------|-------|----------------|----------------|
| \(\cdots\) | \(e\) | \(a\) \((q', b), (q'', a, S)\) | \(f\)          |

Fig. 3. This example shows the corresponding parts of a valid configuration \(C_s\) and its successor configuration \(C_{s+1}\). The previous transition \((q, c), (q', f, L)\) leading to configuration \(C_s\) was reading a \(c \in \Gamma\) on the right cell, writing an \(f \in \Gamma\), switching the state from \(q\) to \(q'\), and finally moving the head one position to the left. The changeover from \(C_s\) to \(C_{s+1}\) was done by using transition \((q', b), (q'', a, S)\), saying reading in state \(q'\) the letter \(b\), write the letter \(a\), switch to state \(q''\), and stay with the head at the current position.

Now, we are ready to describe the structure of the \(r\)-rooted subtrees that encode the configuration; that is the last remaining part of the whole encoding. We already noted that these configuration trees are based on binary trees of height \(n\). Every non root node carries the label \(s\) and Björklund et al. called them skeleton nodes. Every skeleton node has an attached navigation gadget, that is a short path of four nodes labeled by \(p, 0, 1, \perp\) for denoting any children as left children and labeled by \(p, 1, 0, \perp\) for right children in the sequence from the skeleton node to the leaf of the gadget (cf. Figure 2(a)).

Each leaf skeleton node, that is a skeleton node that has no skeleton node as child, carries besides the navigation gadget, a configuration cell gadget that consists of a path of length \(k + 2\). The root node of this path is labeled by \(m\) (for me) followed by \(k\) nodes labeled with digits 0 and 1, and the path ends in a leaf labeled with \(\perp\). \(k - 1\) nodes on this path are labeled with 0, only the \(i\)-th node is labeled by 1, telling the current cell is the cell number \(i\).

To finish the description of the encoding, for technical reasons, we start in the top of the computation tree with a node labeled with \(\top\) that has exactly one child, the topmost configuration node. Now, we are ready to define the ranked

\[^4\text{Recall, } k\text{ is the number of all possible configuration cells of } \mathcal{A}.\]
alphabet $\Sigma'$ and afterwards, to construct the query. The alphabet consists of the following symbols:

- $\top$ of arity $ar(\top) = 1$, that denotes the root node of the encoded computation tree.
- $CT_\forall$ of arity $ar(CT_\forall) = 3$, that denotes a universal configuration.
- $Leaf-CT_\forall$ of arity $ar(Leaf-CT_\forall) = 1$, that denotes a halting configuration, that is a child of an existential configuration.
- $CT_{left}$ of arity $ar(CT_{left}) = 2$, that denotes an existential configuration where the configuration itself is the left child of a universal configuration (or the initial configuration).
- $CT_{right}$ of arity $ar(CT_{right}) = 2$, that denotes an existential configuration where the configuration itself is the right child of a universal configuration.
- $Leaf-CT_{left}$ of arity $ar(Leaf-CT_{left}) = 1$, that denotes a halting configuration where the configuration itself is the left child of a universal configuration (or the initial configuration).
- $Leaf-CT_{right}$ of arity $ar(Leaf-CT_{right}) = 1$, that denotes a halting configuration where the configuration itself is the right child of a universal configuration.
- $r$ of arity $ar(r) = 2$, that denotes the root node of an configuration tree.
- $s$ of arity $ar(s) = 3$, that denotes a skeleton node of an configuration tree.
- $s_{leaf}$ of arity $ar(s_{leaf}) = 2$, that denotes a skeleton leaf node that is a leaf of the configuration tree.
- $p$ of arity $ar(p) = 1$, that denotes the root of an navigation gadget.
- $m$ of arity $ar(m) = 1$, that denotes the root of an cell gadget ‘me’.
- $0$ and $1$ of arity $ar(0) = ar(1) = 1$, for the values of the gadgets.
- $\bot$ the only symbol of $\Sigma_T$ of arity $ar(\bot) = 0$. So every leaf of the encoding tree is labeled by $\bot$.

The construction of the demanded query $Q = (P, Ans)$ starts with a program $P_1$ that ensures the newly introduced idb predicate $structure$ for the root if the input tree $T$ is structured as an encoded computation tree. In particular, the input tree must fulfill the following conditions.

1. The root of the tree is labeled with $\top$ and has exactly one child that represents the initial configuration.
2. Each configuration node has exactly one child labeled with $r$.
3. Every configuration cell gadget correctly encodes a configuration cell.
4. Each encoded configuration tree is complete and has height $n$.
5. Every skeleton node has exactly one correctly assigned navigation gadget.
6. All horizontal constraints from $H(A_w)$ are satisfied.
7. The universal and existential configurations must alternate on the subtree of $CT$ labeled nodes.

5 To be precise, a halting configuration is neither an existential nor a universal configuration, but the labels tell us whose configuration child it is.
For each non halting universal configuration, the two child configuration nodes represent two encoded configuration trees with two different CCells. The highest encoded configuration tree has the start configuration cell
\[ (q_0, ((q_0, S)_0)) \]
as its leftmost configuration cell. Recall, \( q_0 \) is the initial state of \( A_w \) and the computation starts on an empty tape.

Every configuration node that has no successor configuration encodes a final configuration, that implies the leftmost configuration cell is of the form
\[ (a, ((q, b), (q_a, c, m))) \]
Recall \( q_a \) is the accepting state of the machine, the machine, upon accepting, moves its head to the leftmost tape cell, and finally, an input tree is accepted if every path in the computation tree leads to an accepting halting configuration.

The program \( P_1 \) will start in the leaves of the encoded tree and verifies the structure step by step in the direction to the root node. For the beginning, the program \( P_1 \) is the empty set of rules and the first rule we add is to call leaves by what they are. Thus, we add
\[ \text{leaf}(x) \leftarrow \text{label}_1(x). \]
In any case, a leaf belongs to a gadget, that is a cell configuration or a navigation gadget, and therefore we count the length of the digit path up to the length of \( k \) by the following rules.

\[
\begin{align*}
0(x) & \leftarrow \text{label}_0(x) \\
1(x) & \leftarrow \text{label}_1(x) \\
digit(x) & \leftarrow 0(x) \\
digit(x) & \leftarrow 1(x) \\
digit_0(x) & \leftarrow \text{leaf}(x) \\
digit_1(x) & \leftarrow \text{digit}(x), \text{child}(x, y), \text{digit}_0(y) \\
digit_2(x) & \leftarrow \text{digit}(x), \text{child}(x, y), \text{digit}_1(y) \\
& \quad \ldots \\
digit_k(x) & \leftarrow \text{digit}(x), \text{child}(x, y), \text{digit}_{k-1}(y)
\end{align*}
\]

Additionally, to ensure that a navigation gadget and the 'me' cell configuration gadget have exactly one node labeled with 1, we count the amount of 1-labeled nodes on every digit path by the following rules.

\[
\begin{align*}
\text{count}^{1}_{<1}(x) & \leftarrow \text{leaf}(x) \\
\text{count}^{1}_{<1}(x) & \leftarrow 0(x), \text{child}(x, y), \text{count}^{1}_{<1}(y) \\
\text{count}^{1}_{<1}(x) & \leftarrow 1(x), \text{child}(x, y), \text{count}^{1}_{<1}(y) \\
\text{count}^{1}_{<1}(x) & \leftarrow 0(x), \text{child}(x, y), \text{count}^{1}_{<1}(y)
\end{align*}
\]
We propagate this counting results to the gadget roots if they are labeled by \( m \) or \( p \) by adding the following rules to \( P_1 \):

\[
\begin{align*}
\text{count}_{\text{m}1}(x) & \leftarrow \text{label}_{\text{p}}(x), \text{child}(x, y), \text{count}_{\text{m}1}(y) \\
\text{digit}_2(x) & \leftarrow \text{label}_{\text{p}}(x), \text{child}(x, y), \text{digit}_2(x) \\
p(x) & \leftarrow \text{label}_{\text{p}}(x), \text{count}_{\text{m}1}(x), \text{digit}_2(x) \\
\text{count}_{\text{m}1}(x) & \leftarrow \text{label}_{\text{m}}(x), \text{child}(x, y), \text{count}_{\text{m}1}(y) \\
\text{digit}_k(x) & \leftarrow \text{label}_{\text{m}}(x), \text{child}(x, y), \text{digit}_k(x) \\
m(x) & \leftarrow \text{label}_{\text{m}}(x), \text{count}_{\text{m}1}(x), \text{digit}_k(x)
\end{align*}
\]

Now, the predicate \( p \) becomes true for a node \( v \) of the input tree \( T \) if it is labeled with \( p \) and it is the starting node of a navigation gadget that actually denotes a direction, as well as, \( m \) becomes true for a node \( v \) of the input tree \( T \) if it is labeled with \( m \) and it is the starting node of a ‘me’ cell configuration gadget that actually denotes a configuration cell.

For the rest of the section, we introduce a predicate \( \text{child}^i(x, y) \) for a natural number \( i \) as short hand for the set of atoms

\[
\text{child}(x, x_1), \text{child}(x_1, x_2), \ldots, \text{child}(x_{i-1}, y)
\]

where \( \text{child}^i(x, y) \) states the fact that \( y \) is a descendant of \( x \) in the \( i \)-th generation.

By the following rules, every \( m \)-marked node knows which configuration \( i \in \{1, \ldots k\} \) it encodes.

\[
\begin{align*}
m_{k=1}(x) & \leftarrow m(x), \text{child}(x, x_1), 1(x_1) \\
m_{k=2}(x) & \leftarrow m(x), \text{child}^2(x, x_2), 1(x_2) \\
& \vdots \\
m_{k=i}(x) & \leftarrow m(x), \text{child}^i(x, x_i), 1(x_i) \\
& \vdots \\
m_{k=k}(x) & \leftarrow m(x), \text{child}^k(x, x_k), 1(x_k)
\end{align*}
\]

Now, we mark the leaves of the skeleton nodes with the idb predicate \( s_{\text{leaf}} \) that are leaves in the configuration tree considered without the gadgets.

\[
s_{\text{leaf}}(x) \leftarrow \text{label}_{\text{s}_{\text{leaf}}}(x), \text{child}(x, x_m), m(x_m), \text{child}(x, x_p), p(x_p)
\]

Observe, the label \( s_{\text{leaf}} \) has arity two, so there cannot be further children the rule could work on. Now, for the subtrees rooted by nodes marked with \( s_{\text{leaf}} \) the condition (3) is fulfilled. By the next rules, we mark the nodes carrying the label \( s \) or \( s_{\text{leaf}} \) regarding their navigation gadget as left child using \( s_L \) or as right child by using \( s_R \). Remember a correct navigation gadget is marked by the idb
predicate $p$.

\[
    s_L(x) \leftarrow \text{label}_x, \text{child}(x, p(x_p), p(x_p), p(x_n), 0(x_n))
\]

\[
    s_R(x) \leftarrow \text{label}_x, \text{child}(x, p(x_p), p(x_p), p(x_n), 1(x_n))
\]

\[
    s_L(x) \leftarrow \text{label}_x, \text{child}(x, p(x_p), p(x_p), p(x_n), 0(x_n))
\]

\[
    s_R(x) \leftarrow \text{label}_x, \text{child}(x, p(x_p), p(x_p), p(x_n), 1(x_n))
\]

We are going to mark the entire configuration tree with the predicate $s$, that affects the nodes marked by $s_{\text{leaf}}$ and every node labeled by $s$ that have a correct navigation gadget, as well as left and right children.

\[
    s(x) \leftarrow s_{\text{leaf}}(x)
\]

\[
    s(x) \leftarrow s_L(x), \text{child}(x, x_l), s_L(x_l), s(x_l), \text{child}(x, x_r), s_R(x_r), s(x_r)
\]

\[
    s(x) \leftarrow s_R(x), \text{child}(x, x_l), s_L(x_l), s(x_l), \text{child}(x, x_r), s_R(x_r), s(x_r)
\]

Note, an inner node of the configuration tree is itself a left or right child, that implies there is such a navigation gadget and it gets the $s$ predicate, if it has a left and a right child, marked with $s_L$ and $s_R$. This implies, this node cannot own a second navigation gadget that claims the opposite of another navigation gadget since the arity of the symbol $s$ enforces the limit of exactly three children. Remember, we have to ensure that the configuration tree is complete and has height $n$. This will be done if both children of the $r$ labeled root of the configuration tree are marked by height $n-1$ and by $s$ since $s$ is only true for them if every $s$ child itself has two $s$ children down to the leaves of the configuration tree. So, up to $n-1$, we count the height of the configuration tree by adding the following rules to $P_1$.

\[
    s_h=0(x) \leftarrow s_{\text{leaf}}(x)
\]

\[
    s_h=1(x) \leftarrow \text{child}(x, x_l), s_L(x_l), s_h=0(x_l), \text{child}(x, x_r), s_R(x_r), s_h=0(x_r)
\]

\[
    \vdots
\]

\[
    s_h=n-1(x) \leftarrow \text{child}(x, x_l), s_L(x_l), s_h=n-2(x_l), \text{child}(x, x_r), s_R(x_r), s_h=n-2(x_r)
\]

To this end, we mark a node labeled by $r$ with the predicate $r_{\text{nav}}$ if it is the root of a navigable and complete configuration tree and add the rule

\[
    r_{\text{nav}}(x) \leftarrow \text{label}_x, \text{child}(x, x_l), s_L(x_l), s(x_l), s_h=n-1(x_l)
\]

\[
    \text{child}(x, x_r), s_R(x_r), s(x_r), s_h=n-1(x_r)
\]

\[
    \text{to } P_1. \text{ Observe, during the computation of } P_1(T) \text{ a node labeled by } r \text{ gets marked with } r_{\text{nav}} \text{ if it is a root of a complete configuration tree of height } n \text{ where every skeleton node carries a correct navigation gadget and in the skeleton leaves a cell configuration is correctly encoded. So, the conditions } (3) - (5) \text{ are fulfilled.}
\]

The next goal is to ensure condition (6) that stands for the horizontal constraints (H1)–(H3). This actually holds if the tuple $(i, j)$ of two neighboring configurations cells is contained in the relation $H(A_w)$. Remember, a node labeled by $m$ is already marked by $m_{k=i}$ for its encoded configuration $i$. In a first step and for every $i \in \{1, \ldots, k\}$, we propagate this information to the skeleton leaves by the following rules.

\[
    (k = i)_{\text{leaf}}(x) \leftarrow s_{\text{leaf}}(x), \text{child}(x, y), m_{k=i}(y)
\]
Next, we propagate for a subtree of the configuration tree its leftmost and its rightmost configuration cell. Furthermore, it is to verify if the rightmost cell of the left child fits together with the leftmost cell of the right child. Therefore, we use the new predicates \((k = i)_{\text{left}}\) and \((k = i)_{\text{right}}\) for every \(i \in \{1, \ldots, k\}\) in the following rules

\[
\begin{align*}
(k = i)_{\text{left}}(x) & \leftarrow s(x), (k = i)_{\text{leaf}}(x) \\
(k = i)_{\text{right}}(x) & \leftarrow s(x), (k = i)_{\text{leaf}}(x) \\
(k = i)_{\text{left}}(x) & \leftarrow s(x), \text{child}(x, x_l), s_L(x_l), (k = i)_{\text{left}}(x_l) \\
(k = i)_{\text{right}}(x) & \leftarrow s(x), \text{child}(x, x_r), s_R(x_r), (k = i)_{\text{right}}(x_r),
\end{align*}
\]

as well as for every \((i, j) \in H(A_w)\), the predicate \(H\) (if the nodes children fit together) in the following rules

\[
\begin{align*}
H(x) & \leftarrow s(x), \text{child}(x, x_l), s_L(x_l), s_{\text{leaf}}(x_l), (k = i)_{\text{right}}(x_l), \\
& \text{child}(x, x_r), s_R(x_r), s_{\text{leaf}}(x_r), (k = j)_{\text{left}}(x_r) \\
H(x) & \leftarrow s(x), \text{child}(x, x_l), s_L(x_l), H(x_l), (k = i)_{\text{right}}(x_l), \\
& \text{child}(x, x_r), s_R(x_r), H(x_r), (k = j)_{\text{left}}(x_r) \\
H(x) & \leftarrow \text{label}(x), \text{child}(x, x_l), s_L(x_l), H(x_l), (k = i)_{\text{right}}(x_l), \\
& \text{child}(x, x_r), s_R(x_r), H(x_r), (k = j)_{\text{left}}(x_r).
\end{align*}
\]

Now, a node labeled by \(r\) is marked with \(H\) if its configuration tree satisfies all horizontal constraints from \(H(A_w)\). By the following rules, we ensure that in a configuration tree do not exist two different CCells and use the idb predicate \(\theta\) if the CCell \(i\) exists in a subtree and \(\text{Non}_\theta\) if a cell does not belong to CCells. For all \(i \in \{1, \ldots, k\}\) where \(i \in \text{CCells}\), we add the rule

\[
\theta_i(x) \leftarrow (k = i)_{\text{leaf}}(x)
\]

and for all \(j \in \{1, \ldots, k\}\) where \(j \notin \text{CCells}\), we add the rules

\[
\text{Non}_\theta(x) \leftarrow (k = j)_{\text{leaf}}(x)
\]

to \(\mathcal{P}_1\). This will be propagated by

\[
\begin{align*}
\theta_i(x) & \leftarrow \text{child}(x, x_l), s_L(x_l), \theta_i(x_l), \text{child}(x, x_r), s_R(x_r), \text{Non}_\theta(x_r) \\
\theta_i(x) & \leftarrow \text{child}(x, x_l), s_L(x_l), \text{Non}_\theta(x_l), \text{child}(x, x_r), s_R(x_r), \theta_i(x_r)
\end{align*}
\]

for every \(i \in \{1, \ldots, k\}\) where \(i \in \text{CCells}\) and finally, a node labeled by \(r\) carries the idb predicate \(\theta_i\) for exactly one \(i \in \{1, \ldots, k\}\) if its configuration contains exactly one CCell, that is the configuration cell \(i\). Otherwise, the node is not marked by any \(\theta_i\) predicate. Implied by the following rules

\[
r(x) \leftarrow \text{label}(x), H(x), r_{\text{leaf}}(x), \theta_i(x) \quad \text{for all } i \in \text{CCells}
\]

every root node of a configuration tree is marked with \(r\) if its configuration tree satisfies the conditions \((3) - (6)\).

Purposing the bottom-up analysis of the input tree, we have to verify that a configuration node labeled by Leaf-CT\(_{\varphi}\), Leaf-CT\(_{\varphi}^{\text{left}}\), or Leaf-CT\(_{\varphi}^{\text{right}}\) represents a halting configuration that is given as CCell in the leftmost cell of its configuration
tree. So, for all \( i \in \text{CCells} \) representing a configuration cell with current state \( q_a \) that is the only accepting state of \( A_w \), we add the rules

\[
\begin{align*}
\text{Leaf-CT}_v(x) & \leftarrow \text{label}_{\text{Leaf-CT}_v}(x), \text{child}(x, x_r), r(x_r), \theta_i(x_r), (k = i)_{\text{left}}(x_r) \\
\text{Leaf-CT}_{3}^{\text{left}}(x) & \leftarrow \text{label}_{\text{Leaf-CT}_{3}^{\text{left}}}(x), \text{child}(x, x_r), r(x_r), \theta_i(x_r), (k = i)_{\text{left}}(x_r) \\
\text{Leaf-CT}_{3}^{\text{right}}(x) & \leftarrow \text{label}_{\text{Leaf-CT}_{3}^{\text{right}}}(x), \text{child}(x, x_r), r(x_r), \theta_i(x_r), (k = i)_{\text{left}}(x_r)
\end{align*}
\]

Recall, the rank of the symbols representing a halting configuration is \( ar(\text{Leaf-CT}_v) = ar(\text{Leaf-CT}_{3}^{\text{right}}) = ar(\text{Leaf-CT}_{3}^{\text{left}}) = 1 \) and so, for every subtree rooted by a node marked with the latter introduced idb predicates, we ensured conditions \([4] - [9]\) and \([11]\).

It remains to analyze the subtrees of the CT labeled nodes. Recall, an inner node of the CT tree will be positively marked if

(a) it is labeled as universal configuration and it has two existential configuration children (one or both can be a leaf configuration node) carrying different CCells, or

(b) it is labeled as existential configuration and it has exactly one universal configuration child (or one leaf configuration node).

Additionally, it has an \( r \) rooted configuration tree as child and the CCell on the \( r \) node denotes a state of the machine that is existential if the configuration node is labeled as existential or that is universal if the configuration node is labeled as one \(^6\). So, we introduce predicates \( \text{state}_3 \) and \( \text{state}_v \), as well as we extend the handling of the idb-predicates \( \text{Leaf-CT}_v, \text{Leaf-CT}_{3}^{\text{right}}, \) and \( \text{Leaf-CT}_{3}^{\text{left}} \) by the following rules

\[
\begin{align*}
\text{state}_3(x) & \leftarrow r(x), \theta_i(x) \\
\text{state}_v(x) & \leftarrow r(x), \theta_j(x)
\end{align*}
\]

for all \( i \in \text{CCells} \) where \( i \) is a configurations cell of an existential state, and

\[
\begin{align*}
\text{state}_v(x) & \leftarrow r(x), \theta_j(x)
\end{align*}
\]

for all \( j \in \text{CCells} \) where \( j \) is a configurations cell of a universal state, and finally, we add

\[
\begin{align*}
\text{CT}_{3}^{\text{left}}(x) & \leftarrow \text{Leaf-CT}_{3}^{\text{left}}(x) \\
\text{CT}_{3}^{\text{left}}(x) & \leftarrow \text{state}_3(x), \text{label}_{\text{CT}_{3}^{\text{left}}}(x), \text{child}(x, x_r), \text{child}(x, x_a), \text{CT}_v(x_a), \text{CT}_{v}(x_a), \\
\text{CT}_{3}^{\text{right}}(x) & \leftarrow \text{Leaf-CT}_{3}^{\text{right}}(x) \\
\text{CT}_{3}^{\text{right}}(x) & \leftarrow \text{state}_3(x), \text{label}_{\text{CT}_{3}^{\text{right}}}(x), \text{child}(x, x_r), \text{child}(x, x_a), \text{CT}_v(x_a), \text{CT}_v(x_a), \\
\text{CT}_v(x) & \leftarrow \text{Leaf-CT}_v(x) \\
\text{CT}_v(x) & \leftarrow \text{state}_v(x), \text{label}_{\text{CT}_v}(x), \text{child}(x, x_r), \text{child}(x, x_1), \text{CT}_{3}^{\text{left}}(x_1), \text{child}(x_1, x_{1,1}), r(x_{1,1}), \theta_i(x_{1,1}), \\
& \quad \text{child}(x, x_2), \text{CT}_{3}^{\text{right}}(x_2), \text{child}(x_2, x_{2,1}), r(x_{2,1}), \theta_j(x_{2,1})
\end{align*}
\]

\(^6\) Recall, the rank of \( \text{CT}_{3}^{\text{left}}, \text{CT}_{3}^{\text{right}}, \) and \( \text{CT}_v \) is \( ar(\text{CT}_{3}^{\text{left}}) = 2, ar(\text{CT}_{3}^{\text{right}}) = 2, \) and \( ar(\text{CT}_v) = 3.\)
for all \(i \neq j \in \{1, \ldots, k\}\). Observe, that a node \(v\) is marked with \(CT_{left}^{\underline{3}}, CT_{right}^{\underline{3}}\), or \(CT_v\) if its subtree rooted by \(v\) satisfies the conditions \([2] - [8]\) and \([10]\).

Now, to ensure condition \([9]\) we fix \(i \in \mathbb{C}Cells\) that represents the configuration \((\omega((q_0, \omega), (q_0, \omega, S)))\) and add the following rules

\[
\begin{align*}
\text{Start-CT}(x) & \leftarrow CT_v(x), \text{child}(x, x_r, r(x_r), \theta_i(x_r)) \\
\text{Start-CT}(x) & \leftarrow CT_{left}^{\underline{3}}(x), \text{child}(x, x_r, r(x_r), \theta_i(x_r))
\end{align*}
\]

Let \(\mathcal{P}_1\). It is not forbidden that more than one node of the computation tree carries the marker as start configuration node, but the topmost configuration node has to be marked. And therefore, we add the rule

\[
structure(x_\top) \leftarrow \text{label}_\top(x_\top), \text{child}(x_\top, x_{CT}), \text{Start-CT}(x_{CT})
\]

and obtain a program \(\mathcal{P}_1\) such that a query \(Q' = (\mathcal{P}_1, structure)\) yields yes on an input tree \(T\) if and only if \(T\) satisfies conditions \([11] - [10]\), that is, if and only if it is structured as an encoded computation tree of \(\mathbb{A}_w\).

To complete the demanded query \(Q = (\mathcal{P}, Ans)\), it remains to extend the program \(\mathcal{P}_1\) in a way that \(Q\) accepts the tree if the \(structure\) predicate is true for its root and the encoded configurations does not violate the transition relation. For the beginning, let \(\mathcal{P}\) consists of all rules of \(\mathcal{P}_1\). To shorten the query program, we mark all configuration nodes with the predicate CT by adding the following rules.

\[
\begin{align*}
CT(x) & \leftarrow CT_v(x) & \text{Leaf-CT}(x) & \leftarrow \text{Leaf-CT}_v(x) \\
CT(x) & \leftarrow CT_{left}^{\underline{3}}(x) & \text{Leaf-CT}(x) & \leftarrow \text{Leaf-CT}_{left}^{\underline{3}}(x) \\
CT(x) & \leftarrow CT_{right}^{\underline{3}}(x) & \text{Leaf-CT}(x) & \leftarrow \text{Leaf-CT}_{right}^{\underline{3}}(x)
\end{align*}
\]

Since the upcoming rules are very large, we introduce short hands as binary predicates\(^7\) First, we define a predicate \(\text{Succ}(x_{r_1}, x_{r_2})\) that is true for two nodes \(x_{r_1}\) and \(x_{r_2}\) if they are root nodes of successive encoded configuration trees.

\[
\text{Succ}(x_{r_1}, x_{r_2}) := \left\{ r(x_{r_1}), r(x_{r_2}), CT(s_1), CT(s_2), \text{child}(s_1, s_2), \text{child}(s_1, x_{r_1}), \text{child}(s_2, x_{r_2}) \right\}
\]

The next predicate \(\text{SameLevel}_L(x_{s_1}, x_{s_2})\) for an \(i > 0\) states for two nodes \(x_{s_1}\) and \(x_{s_2}\) that they are on the same level \(i\) in the configuration tree of two successive encoded configuration trees.

\[
\text{SameLevel}_L(x_{s_1}, x_{s_2}) := \left\{ s(x_{s_1}), s(x_{s_2}), \text{Succ}(x_{r_1}, x_{r_2}), \text{child}(x_{r_1}, x_{s_1}), \text{child}(x_{r_2}, x_{s_2}) \right\}
\]

The predicate \(\text{SameLevel}_L^{LR}(x_{s_1}, x_{s_2})\) extends the predicate \(\text{SameLevel}_L(x_{s_1}, x_{s_2})\) by the following property: The nodes \(x_{s_1}\) and \(x_{s_2}\) have to be both the left or

\(^7\) This does not mean that our datalog program is no longer a monadic program, in fact, we use these predicates for replacements in the rule to increase the readability of the whole rule. Variables occurring in the definition of the predicate, but not in the head, have to be renamed in a later context if it is necessary.
both the right child of their parent.

\[
\text{SameLevel}^L_R(x_{s_1}, x_{s_2}) := \begin{cases}
\text{SameLevel}_i(x_{s_1}, x_{s_2}), \\
\text{child}(x_{s_1}, x_{p_1}), \text{child}(x_{s_2}, x_{p_2}), p(x_{p_1}), p(x_{p_2}), \\
\text{desc}(x_{p_1}, x_t_1), \text{desc}(x_{p_2}, x_t_2), 1(x_t_1), 1(x_t_2), \\
\text{child}^{i+4}(z, x_t_1), \text{child}^{i+5}(z, x_t_2) 
\end{cases}
\]

Observe, that the node \( z \) is the configuration node of the predecessor configuration or its parent node and so, for the initial configuration at the top of the encoded computation tree, the extra buffering node above is necessary. Furthermore, this is the only point during the reduction where the desc predicate is actually indispensable; we use it to guess whether the nodes are left or right children. In particular, if the nodes \( x_{t_1} \) and \( x_{t_2} \) do not indicate the same left- or right-orientation then the distance to \( z \) is not \( i + 4 \) for the predecessor and \( i + 5 \) for the successor and a valuation of the rule will not be possible. Even another labeling of the encoding tree that tells us directly whether a child is the left or the right one seems to be impossible because it implies a rule for every path through the configuration tree; that leads to \( 2^n \) rules and this would avoid a reduction in time polynomial in \( n \) and the size of the automaton.

Now, we are able to introduce a predicate \( \text{SameCell}(x_{s_1}, x_{s_2}) \) that states for two skeleton nodes \( x_{s_1} \) and \( x_{s_2} \) reflecting the same cell of successive encoded configuration cell sequences; those cells are at depth \( n \) of any configuration tree.

\[
\text{SameCell}(x_{s_1}, y_{s_2}) := \\
\bigcup_{1 \leq i \leq n-1} \{ \text{child}(x_{i}, x_{i+1}), \text{child}(y_{i}, y_{i+1}), \text{SameLevel}^L_R(x_i, y_i) \} \\
\bigcup \{ \text{child}(x_{n-1}, x_{s_1}), \text{child}(y_{n-1}, y_{s_2}), \text{SameLevel}^L_R(x_{s_1}, y_{s_2}) \}
\]

Next, we use the idb predicate \( \delta \) to denote that a configuration cell meshes with its predecessor configuration cell in respect to the transition relation. So, for every tuple \( (i, j) \in V(A_u) \) we add the following rule

\[
\delta(x_{s_j}) \leftarrow \text{SameCell}(x_{s_1}, x_{s_2}), \text{child}(x_{s_1}, x_{m_1}), m(x_{m_1}), m_{k=i}(x_{m_1}), \\
\text{child}(x_{s_2}, x_{m_2}), m(x_{m_2}), m_{k=j}(x_{m_2})
\]

to \( P \). To verify the correctness of this rule, recall that the \( m \)-labeled node \( v \) of an 'me' cell configuration gadget is already marked with \( m_{k=i}(v) \) if its gadget encodes the configuration cell \( i \). Now, we have to verify that every configuration cell of the encoded sequence respects the transition relation regarding its predecessor configuration cell and propagate this information to the configuration node by the following rules.

\[
\delta(x) \leftarrow \text{child}(x, x_l), s_L(x_l), \delta(x_l), \text{child}(x, x_r), s_R(x_r), \delta(x_r) \\
\delta(x) \leftarrow \text{CT}(x), \text{child}(x, x_r), r(x_r), \delta(x_r)
\]

The next step is to collect the information that every configuration node is a valid successor up to the top of the tree and we obtain that a configuration node \( v \) is marked with \( \Delta \) if the subtree rooted at \( v \) is a suffix of a valid computation
Clearly, if the topmost configuration tree is an initial configuration and marked with \( \Delta \) then we know that the input tree represents a valid accepting computation of \( A_w \). To this end, we conclude the construction by adding the rule

\[
\text{Ans}(x) \leftarrow \text{structure}(x), \text{child}(x, x_{\text{CT}}), \Delta(x_{\text{CT}})
\]

and obtain the demanded query \( Q = (\mathcal{P}, \text{Ans}) \) within polynomial time; that finishes the proof of Theorem 6.

\[\Box\]

\section*{B Hardness on Unranked Trees}

\textbf{Theorem 5 (restated)} The QCP for Boolean mDatalog(\( \tau_u^{\text{desc}} \)) on finite labeled unordered trees is \( \text{2EXPTIME-hard} \).

\textit{Proof.} We prove the theorem by using and extending the proof of Theorem \( \Box \) so we establish a reduction from the word acceptance problem of exponential space bounded alternating Turing machines to the QCP for mDatalog(\( \tau_u^{\text{desc}} \)) on unranked labeled unordered trees. More precisely, we give a polynomial time reduction to the complement of the named QCP. For a given ATM \( A_w \) that is normalized and composed of the original ATM \( A \) and its input word \( w \), we construct within polynomial time a finite unranked alphabet \( \Sigma_{\text{ur}} \) and two Boolean mDatalog(\( \tau_u^{\text{desc}}, \Sigma_{\text{ur}} \))-queries \( Q_1 \) and \( Q_2 \), such that

\[
\begin{align*}
w \in L(A) & \iff \text{there is an accepting computation tree for } A_w \\
& \iff \text{there exists an unordered } \Sigma_{\text{ur}}\text{-labeled tree } T \text{ such that } Q_1(T) = \text{yes and } Q_2(T) = \text{no} \\
& \iff Q_1 \not\subseteq Q_2.
\end{align*}
\]

Recall the reduction from Theorem \( \Box \) the utilized ranked alphabet \( \Sigma' \), and the obtained program \( \mathcal{P} \) in mDatalog(\( \tau_u^{\text{desc}} \)) on ranked trees. We choose the unranked alphabet \( \Sigma_{\text{ur}} \) as the unranked version of \( \Sigma' \), to be precise we set \( \Sigma_{\text{ur}} := \{ \alpha | \alpha \in \Sigma' \} \). Furthermore, we set \( Q_1 := (\mathcal{P}, \text{Ans}) \), that is, the query constructed during the former reduction. So, \( Q_1 \) stands for the ”necessary properties” of the encoded computation tree. Since the alphabet is no longer ranked, we cannot avoid that a node has more than the planned children, but we can forbid that the redundant children have other labels and falsify the computation. Therefore, all that remains is to construct a query \( Q_2 \) in mDatalog(\( \tau_u^{\text{desc}} \)) such that \( Q_2 \)
describe "forbidden properties". A tree with such properties does not describe an encoded computation tree. To this end, we check for forbidden labels on child nodes, a child of an s-labeled node, for example, must not be labeled with CT\(_v\), and we have to test that there are no two paths encoding inconsistent information. Thus, the query \( Q_2 = (P_2, \text{reject}) \) will yield to yes on an input tree if at least one of the following facts are true.

(1) A non root node is labeled by \( \top \).
(2) The root has a child that is not labeled by an CT-label.
(3) A non halting existential configuration node has a child labeled with a symbol not in \{r, CT\(_v\), Leaf-CT\(_v\)\}.
(4) An non halting universal configuration node has a child labeled with a symbol not in \{r, CT\(_3^{\text{right}}\), CT\(_3^{\text{left}}\), Leaf-CT\(_3^{\text{right}}\), Leaf-CT\(_3^{\text{left}}\)\}.
(5) A halting configuration node has a child labeled with a symbol that is not \( r \).
(6) An \( r \) labeled node has a child labeled with a symbol that is not \( s \).
(7) An \( s \) labeled node has a child labeled with a symbol not in \{p, s, s\_leaf\}.
(8) An \( s\_\text{leaf} \) labeled node has a child labeled with a symbol not in \{p, m\}.
(9) A \( p \) or \( m \) labeled node has a child labeled with a symbol not in \{0, 1\}.
(10) A 0 or 1 labeled node has a child labeled with a symbol not in \{0, 1, \( \bot \)\}.
(11) A \( \bot \) labeled node has a child.
(12) A \( p \) (or an \( m \)) labeled node has a descendant that is labeled \( \bot \) with distance not equal to three (not equal to \( k + 1 \)), or is not a prefix of a valid gadget.
(13) There exists a path in a configuration tree from the \( r \) labeled node to an \( s\_\text{leaf} \) of length not equal to \( n \).
(14) If any node has two children fulfilling the same role, but encoding different information.

Obviously, the conditions (1) – (13) reflect the underlying structure. Additionally, an illustration to condition (12) is given with Figure 4 (a). Condition (14) reflects the consistence of the encoding and enforces the following: if there are two configurations as children of a node in the computation tree, both universal, both left – or right – existential, then they have to provide exactly the same information during the computation. This includes the contained configuration trees, navigation gadgets, and so on, which can have different copies or copies of prefixes. Intuitively, it is clear that it does not matter if a node has additional children, but they must not provide wrong information; since every rule uses a maximum distance of \( 3 + n + k \), it suffices to have a fixed look ahead inside the encoded configuration (cf. Figure 4 (b)). Now, it is comprehensible that the query \( Q_2 \) fulfilling condition (1)–(14) yields no on a tree \( T \) and \( Q_1 \) yields yes on the same tree if and only if \( T \) is an encoded accepting computation of \( A_w \).

For the beginning, let \( P_2 \) consist of all rules of \( P \). We only consider trees \( T \) with \( Q_1(T) = \text{yes} \), otherwise we have in any way \( Q_1 \leq Q_2 \), which is enough for the reduction. To propagate any detected violation to the root node of the input tree, we propagate the \text{reject} predicate from any node to the root by adding the following rule

\[
\text{reject}(x) \leftarrow \text{child}(x, x_1), \text{reject}(x_1)
\]
Fig. 4. (a) An example of allowed "extentions" of the encoded computation tree, considered at a navigation gadget that can exist multiple times where a copy also can be reduced to a prefix. (b) If the nodes marked by $m_k=i$ and $m_k=j$ have the same path through their configuration tree, that is, the same sequence of left and right children, then $i$ must be equal to $j$.

to $P_2$. We reflect condition $\mathcal{I}$ by adding the rule

$$\text{reject}(x) \leftarrow \text{child}(x, x_1), \text{label}_\top(x_1).$$

Since $Q_1(T) = \text{yes}$, we know the root is labeled with $\top$ and so, we mirror condition $\mathcal{I}$ by the rule

$$\text{reject}(x) \leftarrow \text{label}_\top(x), \text{child}(x, x_1), \text{label}_\alpha(x_1)$$

for every $\alpha \in \Sigma_{wp} \setminus \{CT_T, CT_{left}, CT_{right}\}$.

To verify condition $\mathcal{I}$ we add the rules

$$\text{reject}(x) \leftarrow \text{label}_{CT_{left}}(x), \text{child}(x, x_1), \text{label}_\alpha(x_1)$$

$$\text{reject}(x) \leftarrow \text{label}_{CT_{right}}(x), \text{child}(x, x_1), \text{label}_\alpha(x_1)$$

for every $\alpha \in \Sigma_{wp} \setminus \{r, CT_T, \text{Leaf-CT}_T\}$.

To verify condition $\mathcal{I}$ we add the rule

$$\text{reject}(x) \leftarrow \text{label}_{\text{Leaf-CT}_T}(x), \text{child}(x, x_1), \text{label}_\alpha(x_1)$$

for every $\alpha \in \Sigma_{wp} \setminus \{r, CT_{left}, CT_{right}, \text{Leaf-CT}_{left}, \text{Leaf-CT}_{right}\}$.

To verify condition $\mathcal{I}$ we add the rules

$$\text{reject}(x) \leftarrow \text{label}_{\text{Leaf-CT}_T}(x), \text{child}(x, x_1), \text{label}_\alpha(x_1)$$

$$\text{reject}(x) \leftarrow \text{label}_{\text{Leaf-CT}_{right}}(x), \text{child}(x, x_1), \text{label}_\alpha(x_1)$$

for every $\alpha \in \Sigma_{wp} \setminus \{r\}$.

To verify condition $\mathcal{I}$ we add the rule

$$\text{reject}(x) \leftarrow \text{label}_{r}(x), \text{child}(x, x_1), \text{label}_\alpha(x_1)$$

for every $\alpha \in \Sigma_{wp} \setminus \{s\}$.

To verify condition $\mathcal{I}$ we add the rule

$$\text{reject}(x) \leftarrow \text{label}_{s}(x), \text{child}(x, x_1), \text{label}_\alpha(x_1)$$
for every \( \alpha \in \Sigma_{ur} \setminus \{p, s, s_{\text{leaf}}\} \).

To verify condition (9) we add the rule

\[
\text{reject}(x) \leftarrow \text{label}_{s_{\text{leaf}}}(x), \text{child}(x, x_1), \text{label}_\alpha(x_1)
\]

for every \( \alpha \in \Sigma_{ur} \setminus \{p, m\} \).

To verify condition (10) we add the rules

\[
\begin{align*}
\text{reject}(x) & \leftarrow \text{label}_p(x), \text{child}(x, x_1), \text{label}_\alpha(x_1) \\
\text{reject}(x) & \leftarrow \text{label}_m(x), \text{child}(x, x_1), \text{label}_\alpha(x_1)
\end{align*}
\]

for every \( \alpha \in \Sigma_{ur} \setminus \{0, 1\} \).

To verify condition (11) we add the rule

\[
\text{reject}(x) \leftarrow \text{label}_\bot(x), \text{child}(x, x_1)
\]

To verify condition (12), we assume that conditions (9) and (10) are not fulfilled. This implies, the only possible labels at nodes descending a node labeled with \( p \) or \( m \) are 0, 1, and \( \bot \). So, we add the following rules that ensures that no leaf labeled path exists that is too short or too long, that is a path with a node labeled with 0 or 1 on position three for a navigation gadget and on position \( k + 1 \) for a 'me' cell gadget. Thus, we add for the navigation gadget the following rules

\[
\begin{align*}
\text{reject}(x) & \leftarrow \text{label}_p(x), \text{child}(x, x_1), \text{label}_\bot(x_1) \\
\text{reject}(x) & \leftarrow \text{label}_p(x), \text{child}^2(x, x_1), \text{label}_\bot(x_1) \\
\text{reject}(x) & \leftarrow \text{label}_p(x), \text{child}^3(x, x_1), \text{label}_0(x_1) \\
\text{reject}(x) & \leftarrow \text{label}_p(x), \text{child}^3(x, x_1), \text{label}_1(x_1)
\end{align*}
\]

and for the 'me' gadget, we add

\[
\begin{align*}
\text{reject}(x) & \leftarrow \text{label}_m(x), \text{child}(x, x_1), \text{label}_\bot(x_1) \\
\text{reject}(x) & \leftarrow \text{label}_m(x), \text{child}^2(x, x_1), \text{label}_\bot(x_1) \\
& \vdots \\
\text{reject}(x) & \leftarrow \text{label}_m(x), \text{child}^k(x, x_1), \text{label}_\bot(x_1) \\
\text{reject}(x) & \leftarrow \text{label}_m(x), \text{child}^{k+1}(x, x_1), \text{label}_0(x_1) \\
\text{reject}(x) & \leftarrow \text{label}_m(x), \text{child}^{k+1}(x, x_1), \text{label}_1(x_1)
\end{align*}
\]

Recall, \( \text{child}^i(x, y) \) is a short hand for the set of atoms denoting \( y \) as a descendant of \( x \) in the \( i \)-th generation.

By the same way, we reflect condition (13) which says that there exists a path in a configuration tree from the \( r \) labeled node to an \( s_{\text{leaf}} \) of length not equal to \( n \). We know by conditions (6), (7), (9) – (11) that it suffices to test if
there is a shorter path ending on an \( s_{\text{leaf}} \) labeled node, or if there exists a path of length \( n \) ending with an \( s \) labeled node. Therefore, we add the rules

\[
\text{reject}(x) \leftarrow \text{label}_{p}(x), \text{child}(x, x_1), \text{label}_{s_{\text{leaf}}}(x_1)
\]

\[
\text{reject}(x) \leftarrow \text{label}_{r}(x), \text{child}^2(x, x_1), \text{label}_{s_{\text{leaf}}}(x_1)
\]

\[
\vdots
\]

\[
\text{reject}(x) \leftarrow \text{label}_{r}(x), \text{child}^{n-1}(x, x_1), \text{label}_{s_{\text{leaf}}}(x_1)
\]

\[
\text{reject}(x) \leftarrow \text{label}_{r}(x), \text{child}^{n}(x, x_1), \text{label}_{s}(x_1)
\]

to \( \mathcal{P}_2 \).

Finally, we consider condition (14) and we start by verifying all neighboring navigation gadgets. By condition (12) we already know every navigation gadget is a valid navigation gadget or the prefix thereof. By the following rules, we detect if they are in conflict.

\[
\text{reject}(x) \leftarrow \text{child}(x, x_{p_1}), \text{child}(x, x_{p_2}), \text{label}_{p}(x_{p_1}), \text{label}_{p}(x_{p_2}),
\]

\[
\text{child}(x_{p_1}, x_1), \text{child}(x_{p_2}, x_0), \text{label}_{0}(x_0)
\]

\[
\text{reject}(x) \leftarrow \text{child}(x, x_{p_1}), \text{child}(x, x_{p_2}), \text{label}_{p}(x_{p_1}), \text{label}_{p}(x_{p_2}),
\]

\[
\text{child}^2(x_{p_1}, x_1), \text{child}^1(x_1), \text{child}^2(x_{p_2}, x_0), \text{label}_{0}(x_0)
\]

The same holds for the 'me' cell configuration gadget and therefore, we add the rules

\[
\text{reject}(x) \leftarrow \text{child}(x, x_{m_1}), \text{child}(x, x_{m_2}), \text{label}_{m}(x_{m_1}), \text{label}_{m}(x_{m_2}),
\]

\[
\text{child}(x_{m_1}, x_1), \text{child}(x_{m_2}, x_0), \text{label}_{0}(x_0)
\]

\[
\text{reject}(x) \leftarrow \text{child}(x, x_{m_1}), \text{child}(x, x_{m_2}), \text{label}_{m}(x_{m_1}), \text{label}_{m}(x_{m_2}),
\]

\[
\text{child}^2(x_{m_1}, x_1), \text{child}^1(x_1), \text{child}^2(x_{m_2}, x_0), \text{label}_{0}(x_0)
\]

\[
\vdots
\]

\[
\text{reject}(x) \leftarrow \text{child}(x, x_{m_1}), \text{child}(x, x_{m_2}), \text{label}_{m}(x_{m_1}), \text{label}_{m}(x_{m_2}),
\]

\[
\text{child}^k(x_{m_1}, x_1), \text{label}_{1}(x_1), \text{child}^k(x_{m_2}, x_0), \text{label}_{0}(x_0)
\]

Now, we are going to compare the configurations; that will be done analogously to the definition of the short hand predicate SameCell in the previous proof, but without the offset that was used to reach the successor configuration. So, we first define the predicates \( \text{EquiLevel}, \text{EquiLevel}^{LR} \), and \( \text{EquiCell} \), stating that two nodes are in the equivalent level, are both a left or both a right child, and, by the latter, denote equivalent cells.

\[
\text{EquiLevel}_{1}(x_{s_1}, x_{s_2}) := \left\{ \begin{array}{c}
\text{child}(x, x_{r_1}), \text{child}(x, x_{r_2}), r(x_{r_1}), r(x_{r_2}), \\
\text{child}(x_{r_1}, x_{s_1}), \text{child}(x_{r_2}, x_{s_2}), s(x_{s_1}), s(x_{s_2})
\end{array} \right\}
\]

The predicate \( \text{EquiLevel}^{LR}_{1}(x_{s_1}, x_{s_2}) \) extends the predicate \( \text{EquiLevel}_{1}(x_{s_1}, x_{s_2}) \) by the following property: The nodes \( x_{s_1} \) and \( x_{s_2} \) have to be both the left or
both the right child of their parent.

\[
\text{EquiLevel}^\text{LR}_i(x_s, x_s') := \begin{cases}
\text{EquiLevel}^\text{LR}_i(x_s, x_s'), \\
\text{child}(x_s, x_{p_1}), p(x_{p_1}), \text{child}(x_s, x_{p_2}), p(x_{p_2}), \\
\text{desc}(x_{p_1}, x_{t_1}), \text{desc}(x_{p_2}, x_{t_2}), 1(x_{t_1}), 1(x_{t_2}) \\
\text{child}^{i+4}(z, x_{t_1}), \text{child}^{i+4}(z, x_{t_2})
\end{cases}
\]

And finally, we define EquiCell that is true for two nodes denoting configuration cells that encode the same cell of the automaton. Note, that the predicate is reflexive.

\[
\text{EquiCell}(x_s, y_s) := \bigcup_{1 \leq i \leq n-1} \left\{ \text{child}(x_i, x_{i+1}), \text{child}(y_i, y_{i+1}), \text{EquiLevel}^\text{LR}_i(x_i, y_i) \right\}
\]

\[
\cup \left\{ \text{child}(x_{n-1}, x_s), \text{child}(y_{n-1}, y_s), \text{EquiLevel}^\text{LR}_n(x_s, y_s) \right\}
\]

To verify the value \(k\), we utilize the predicate \(m_k\) for every \(i \in \{1, \ldots, k\}\) given by a positive evaluation of query \(Q_1\), and compare them for every \(i, j \in \{1, \ldots, k\}\) with \(i \neq j\) by the following rules

\[
\text{reject}(x) \leftarrow \text{type}(x_{CT_1}), \text{type}(x_{CT_2}), \text{child}^{n+1}(x_{CT_1}, x_s), \text{child}^{n+1}(x_{CT_2}, x_s), \\
\text{EquiCell}(x_s, x_s'), \text{child}(x_s, x_{m_1}), m(x_{m_1}), m_k(x_{m_1}), \\
\text{child}(x_s, x_{m_2}), m(x_{m_2}), m_k(x_{m_2})
\]

for every type \(\in \{CT_1, \text{Leaf-CT}_1, CT_2^{\text{left}}, \text{Leaf-CT}_2^{\text{left}}, CT_2^{\text{right}}, \text{Leaf-CT}_2^{\text{right}}\}\).

Now, it is ensured that two configurations in the same role, provide different information, so the demanded query is defined by \(Q_2 = (P_2, \text{reject})\).

Observe, by \(Q_1\) we evaluate the computation tree by starting in the halting configurations, so it does not matter if a configuration has a successor configuration twice or if these successor configurations themselves have different successor configurations. In this case it suffices if one subtree leads to accepting configurations on the leaves of an appropriate subtree.

\(\square\)