Controlling the Depth, Size, and Number of Subtrees for Two-variable Logic on Trees

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Abstract. Verification of properties of first order logic with two variables $\text{FO}^2$ has been investigated in a number of contexts. Over arbitrary structures it is known to be decidable with $\text{NEXPTIME}$ complexity, with finitely satisfiable formulas having exponential-sized models. Over word structures, where $\text{FO}^2$ is known to have the same expressiveness as unary temporal logic, the same properties hold. Over finite labelled ordered trees $\text{FO}^2$ is also of interest: it is known to have the same expressiveness as navigational XPath, a common query language for XML documents. Prior work on XPath and $\text{FO}^2$ gives a $2\text{EXPTIME}$ bound for satisfiability of $\text{FO}^2$. In this work we give the first in-depth look at the complexity of $\text{FO}^2$ on trees, and on the size and depth of models. We show that the doubly-exponential bound is not tight, and neither do the $\text{NEXPTIME}$-completeness results from the word case carry over: the exact complexity varies depending on the vocabulary used, the presence or absence of a schema, and the encoding used for labels. Our results depend on an analysis of subformula types in models of $\text{FO}^2$ formulas, including techniques for controlling the number of distinct subtrees, the depth, and the size of a witness to finite satisfiability for $\text{FO}^2$ sentences over trees.

1 Introduction

The complexity of verifying properties over a class of structures depends on both the specification language for properties and the class of structures. Full first-order logic (FO) has non-elementary complexity even when applied to very restricted structures – e.g. words. The two-variable fragment of FO, $\text{FO}^2$, is known to have better properties. Satisfiability over arbitrary relational vocabularies is decidable, and satisfiable sentences have exponential-sized models [GKV97]. Over words witness models can also be taken to be exponential, and the satisfiability problem is known to be $\text{NEXPTIME}$-complete, as it is over general structures [EVW02]. The satisfiability results over words extend to give bounds on many related verification problems [BLW12].

The $\text{NEXPTIME}$-completeness of $\text{FO}^2$ over both general structures and word structures raises the question of the impact of structural restrictions on analysis problems for $\text{FO}^2$. Surprisingly the complexity of satisfiability for $\text{FO}^2$ on a class of structures satisfying a very simple graph-theoretic restriction – namely, finite trees – has not been investigated in detail. $\text{FO}^2$ over trees is known to correspond precisely to the navigational core of the XML query language XPath [MdR04], and the satisfiability problem for XPath is known to be complete for $\text{EXPTIME}$; given
that the translation from FO$^2$ to XPath is known to be exponential \cite{MdR04},
this gives a 2EXPTIME bound on satisfiability for FO$^2$ over trees.

In this work we will consider the satisfiability problem for FO$^2$ over finite
trees, and the corresponding question of the size and depth needed for witness
models. In particular, we will consider:

– satisfiability in the presence of all navigational predicates – predicates for
  the parent/child relation, its transitive closure the descendant relation, the
  left- and right- sibling relations and their transitive closures
– the impact on the complexity of limiting sentences to make use of predicates
  in a particular subset.
– satisfiability over general unranked trees, and satisfiability in the presence of
  a schema
– satisfiability over trees where nodes labels are denoted with explicit unary
  labels versus the case where node labels are boolean combinations over
  a propositional alphabet.

We will show that each of these variations impacts the complexity of the
problem. In the process, we will show that the tree case differs in a number of
important ways from that of words. First, the complexity of satisfiability no longer
matches that of FO$^2$ on general structures – it is EXPSPACE-complete. Secondly,
the basic technique for analyzing FO$^2$ on words \cite{EVW02} – bounds on the number
of quantifier-rank types that occur in a structure – is not useful for getting
tight bounds on FO$^2$ over trees. Instead we will use a combination of methods,
including reductions to XPath, bounds on the number of subformula-based types,
and a quotient construction that is based not only on types, but on a set of
distinguished witness nodes. These techniques allow us to distinguish situations
where satisfiable FO$^2$-formulas have models of (reasonably) small depth, and
situations where they have models of small size. This allows us to get a full
picture of the complexity of FO$^2$ satisfiability problems on trees.

Related work. Two-variable logic on data trees – trees where nodes are
associated with values in an infinite set– has been studied by Bojanczyk et. al.
\cite{BMSS09}: there the main result is decidability over the signature with data
equality and the child relation. Figueira’s manuscript \cite{Fig12} considers two-
variable logic with the successor relations corresponding to two linear orders,
which is quite different from considering the two successor relations derived from
a tree order. Kieronski et. al. show that two-variable logic over two transitive
relations is undecidable. The complexity of two-variable logic over ordinary trees
is explicitly studied only in \cite{BK09}, where it is (incorrectly, as we show) stated
that the complexity of satisfiability remains in NEXPTIME for full two-variable
logic.

Organization: Section 2 gives preliminaries. Section 3 gives precise bounds
for the satisfiability of full FO$^2$ on trees. Section 4 considers the case where the
child predicate is absent, while Section 5 considers the case where the descendant
predicate is absent. Section 6 gives conclusions.
2 Logics and Models

We will always use the term “tree” to denote a finite ordered labelled tree, where the labels are sets of unary predicates $P_1 \ldots P_n$. An ordered tree will consist of a finite set of nodes, a directed edge relation $\text{ParentOf}$ between nodes such that the underlying graph forms a tree in the usual sense, a mapping of each $P_i$ to a subset of the nodes, and a sibling relation $\text{NextSib}$ between nodes that forms the successor relation of a linear order when restricted to the set of children of a given node. We sometimes write $m \text{DescOf} n$ to denote that node $m$ is a descendant of node $n$ in a tree, and similarly write $m \text{ChildOf} n$ to denote that $m$ is a child of $n$. A tree satisfies the unary alphabet restriction (UAR) if exactly one $P_i$ holds of each node; in such a tree the labels are just predicates. Given a tree $t$ and node $n$, $\text{SubTree}(t, n)$ denotes the subtree of $t$ rooted at $n$.

We consider first-order logic sentences in which every subformula has at most two variables, allowing the equality predicate as well as relations from the following signatures for trees:

- for general ordered trees, we consider by default a signature $V_{\text{full}}$ containing predicates for the node predicates $P_i$, as well as for the $\text{ParentOf}$ relation, its transitive closure $\text{AncOf}$, the $\text{LeftSibOf}$ relation that holds of $c$ and $d$ if $c$ is the immediate left sibling of $d$, and its transitive closure $\text{LeftOf}$.
- we let $V_{\text{noAncOf}}$ be the vocabulary obtained by removing the descendant relation, $V_{\text{parOf}}$ be the vocabulary obtained by removing all binary relations other than $\text{ParentOf}$, $V_{\text{noParOf}}$ be the vocabulary obtained by removing the $\text{ParentOf}$ relation, and $V_{\text{ancOf}}$ be the vocabulary obtained by removing all binary relations other than $\text{AncOf}$.

We consider $k$-ranked trees as a particular class of unranked trees, and thus can ask whether an FO$^2$ sentence in any of the signatures above is true on a ranked tree. Note that for $k$-ranked trees it is natural to consider signatures that include the relation $\text{ParentOf}_i$, connecting a node to its $i^{th}$ child for each $i \leq k$, either in place of or in addition to the predicates above. We will not consider a separate signature for ranked trees, since it is easy to derive tight bounds for ranked trees for such signatures based on the techniques introduced here. Although we allow equality in our upper bounds, it will not play any role in the lower bounds.

The signatures above used predicates for which the first argument is either higher up in the tree than the second argument ($\text{ParentOf}(c,d)$ means that $c$ is the parent of $d$) or to the left of the second argument. However, in first-order logic, as well as in two-variable first-order logic, we can express the inverse of any atomic relation as a formula. Thus we can use formulas $x \text{DescOf} y$, $x \text{ChildOf} y$, etc. with the obvious meaning (e.g. $x \text{DescOf} y$ meaning $\text{AncOf}(y,x)$). For any vocabulary $V$ above, we let $\text{FO}^2(V)$ denote the fragment of first-order logic consisting of formulas such that every subformula uses at most two variables. When $V$ is omitted it is assumed to be $V_{\text{full}}$.

A ranked tree schema consists of a bottom-up tree automaton on trees of some rank $k$ [Tho97]. A tree automaton takes trees labeled from a finite set $\Sigma$. We will thus identify the symbols in $\Sigma$ with predicates $P_i$, and thus all trees satisfying the schema will satisfy the UAR.
We consider the following problems:

– Given an FO$^2$ sentence $\varphi$ and a schema $S$, determine whether $\varphi$ is satisfied by some tree satisfying $S$. We consider the combined complexity in the formula and schema.

– Given an FO$^2$ sentence $\varphi$, determine if there is some tree (resp. $k$-ranked, unary alphabet tree) that satisfies it.

Some of our results will go through XPath, a common language used for querying XML documents viewed as trees. The navigational core of XPath is a modal language, analogous to unary temporal logic on trees, denoted NavXP. NavXP is built on binary modalities, referred to as axis relations. We will focus on the following axes: self, child, descendant, descendant-or-self, ancestor-or-self, next-sibling, following-sibling, preceding-sibling, previous-sibling. In a tree $t$, we associate each axis $a$ with a set $R_t(a)$ of pairs of nodes. $R_t(child)$ denotes the set of pairs of nodes $(x, y)$ in $t$ where $y$ is a child of $x$, and similarly for the other axes (see [Mar04]).

NavXP consists of path expressions, which denote binary relations between nodes in a tree, and filters, denoting unary relations. Below we give the syntax (from [BK09]), using $p$ to range over path expressions and $q$ over filters.

$L$ ranges over symbols for each labelling of a node (i.e. for general trees, boolean combinations of predicates $P_1 \ldots P_n$, for UAR trees a single predicate).

\[
p ::= \text{step} \mid p/p \mid p \cup p
\]

\[
q ::= p \mid \text{lab}() = L \mid q \land q \mid q \lor q \mid \neg q
\]

where axis relations are given above.

The semantics of NavXP path expressions relative to a tree $t$ is given by:

1. $[\text{axis}] = R^t_a$
2. $[\text{step}[q]] = \{(n, n') \in [\text{step}] : n' \in [q]\}$
3. $[p_1/p_2] = \{(n, n') : \exists w(n, w) \in [p_1] \land (w, v) \in [p_2]\}$
4. $[p_1 \cup p_2] = [p_1] \cup [p_2]$.

For filters we have:

1. $[\text{lab}()] = L = \{n : n \text{ has label } L\}$
2. $[\neg q] = \{n : n \notin [q]\}$
3. $[q_1 \land q_2] = [q_1] \cap [q_2]$.
4. $[\neg q](n) = \{n : n \notin [q]\}$.

A NavXP filter is said to hold of a tree if it holds of the root under the above semantics.

Marx and De Rijke showed an expressive equivalence of NavXP and FO$^2$.

**Proposition 1.** [MdR04] There is an exponential translation from FO$^2$ to NavXP with all axis and from FO$^2[V\text{ancOf}]$ to NavXP with only the descendant and ancestor axes.

Marx has shown that NavXP has an exponential time satisfiability problem [Mar04]. From this and the above proposition, we get the following (implicit in [MdR04]):

**Corollary 1.** The satisfiability problem for FO$^2$ is in 2EXPTIME.

### 3 Satisfiability for full FO$^2$

**Subformula types and exponential depth bounds.** In the analysis of satisfiability of FO$^2$ for words of Etessami, Vardi, and Wilke [EVW02], a NEXPTIME bound is achieved by showing that any sentence with a finite model has a model
of at most exponential size. The small model property follows, roughly speaking, from the fact that any model realizes only exponentially many “quantifier-rank types” – maximal consistent sets of formulas of a given quantifier rank – and the fact that two nodes with the same quantifier-rank type can be identified.

In the case of trees, this approach breaks down in several places. It is easy to see that one cannot always obtain an exponential-sized model, since a sentence can enforce binary branching and exponential depth. Because there are doubly-exponentially many non-isomorphic small-depth subtrees, there can be doubly-exponentially many quantifier-rank types realized even along a single path in a tree: so quantifier-rank types can not be used even to show an exponential depth bound. We thus use subformula types of a given FO²-formula \( \varphi \) (for short, \( \varphi \)-types) – these are maximal consistent collections of one-variable subformulas of \( \varphi \). The \( \varphi \)-type of a node \( n \) in a tree, \( T_{\varphi}(n) \), is defined as the set of subformulas of \( \varphi \) it satisfies. The number of \( \varphi \)-types is only exponential in \( |\varphi| \), but subformula types are more delicate than quantifier-rank types. E.g. nodes with the same \( \varphi \)-type cannot always be identified without changing the truth of \( \varphi \). Most of the upper bounds will be concerned with handling this issue, by adding additional conditions on nodes to be identified, and/or preserving additional parts of the tree.

**Upper bounds for FO².** We exhibit the issues arising and techniques used to solve them by giving an upper bound for the full logic, FO², which improves on the \( 2\text{EXPTIME} \) bound one obtains via translation to modal logic.

**Theorem 1.** The satisfiability problem for FO² is in \( \text{EXPSpace} \).

The key to the proof is to show the “exponential depth property”:

**Lemma 1.** Every satisfiable FO² sentence \( \varphi \) has a model \( T' \) where the depth is bounded by \( 2^{\text{poly}(|\varphi|)} \), and similarly for satisfiability w.r.t UAR trees or ranked schemas. The outdegree of nodes can also be bounded by \( 2^{\text{poly}(|\varphi|)} \).

We give the argument for the depth bound, leaving the similar proof for the branching bound to the appendix. Given a tree \( t \) and nodes \( n_0 \) and \( n_1 \) in \( t \) with \( n_1 \) not an ancestor of \( n_0 \), the overwrite of \( n_0 \) by \( n_1 \) in \( t \) is the tree \( t(n_1 \rightarrow n_0) \) formed by replacing the subtree of \( n_0 \) with the subtree of \( n_1 \) in \( t \). Let \( F \) be the binary relation relating a node \( m \) in \( t \) to its copies in \( t(n_1 \rightarrow n_0) \): \( n_1 \) and its descendants have a single copy if \( n_1 \) is a descendant of \( n_0 \), and two copies otherwise; nodes in \( \text{SubTree}(t, n_0) \) that are not in \( \text{SubTree}(t, n_1) \) have no copies, and other nodes have a single copy. In the case that \( n_1 \) is a descendant of \( n_0 \), \( F \) is a partial function. We say an equivalence relation \( \equiv \) on nodes of a tree \( t \) is globally \( \varphi \)-preserving if for any equivalent nodes \( n_0, n_1 \) in \( t \) with \( n_0 \notin \text{SubTree}(t, n_1) \), the \( \varphi \)-type of a node \( n \) in \( t \) is the same as the \( \varphi \)-type of nodes in \( F(n) \) within \( t(n_1 \rightarrow n_0) \). We say it is pathwise \( \varphi \)-preserving if this holds for any node \( n_0, n_1 \) in \( t \) with \( n_1 \) a descendant of \( n_0 \). The path-index of an equivalence relation on \( t \) is the maximum of the number of equivalence classes represented on any path, while the index is the total number of classes.

We can not always overwrite a node with another having the same \( \varphi \)-type, but by adding additional information, we can get a pathwise \( \varphi \)-preserving relation
with small path-index. For a node $n$, let $\text{DescTypes}(n)$ be the set of $\varphi$-types of descendants of $n$, and $\text{AncTypes}(n)$ the set of $\varphi$-types of ancestors of $n$. Let $\text{IncompTypes}(n)$ be the $\varphi$-types of nodes $n'$ that are neither descendants nor ancestors of $n$. Say $n_0 \equiv_{\text{Full}} n_1$ if they agree on their $\varphi$-type, the set $\text{DescTypes}$, the set $\text{AncTypes}$, and the set $\text{IncompTypes}$.

**Lemma 2.** The relation $\equiv_{\text{Full}}$ is pathwise $\varphi$-preserving, and its path index is bounded by $2^{\text{poly}(|\varphi|)}$. Thus, there is a polynomial $P$ such that for any tree $t$ satisfying $\varphi$ and root-to-leaf path $p$ of length at least $2^P(|\varphi|)$, there are two nodes $n_0, n_1$ on $p$ such that $t(n_1 \rightarrow n_0)$ still satisfies $\varphi$. Given a tree automaton $A$, it can be arranged that $A$ reaches the same state on $n_0$ as on $n_1$.

Given Lemma 2, Lemma 1 follows by contracting all paths exceeding a given length until the depth of the tree is exponential in $|\varphi|$. In fact (e.g., for ranked trees) $\equiv_{\text{Full}}$ can be used as the state set of a tree automaton. The path index property implies that the automaton goes through only exponentially many states on any path of a tree. By taking the product of this automaton with a ranked schema, the corresponding depth bound relative to a schema follows.

We give the simple argument for the path index bound in Lemma 2 leaving the proof that $\equiv_{\text{Full}}$ is pathwise $\varphi$-preserving to the appendix. First, note that the total number of $\varphi$-types is exponential in $|\varphi|$. Now the sets $\text{DescTypes}(n)$ either become smaller or stay the same as $n$ varies down a path, and hence can only change exponentially often. Similarly the sets $\text{IncompTypes}(n)$ and $\text{AncTypes}(n)$ grow bigger or stay the same, and thus can change only exponentially often.

In intervals along a path where both of these sets are stable, the number of possibilities for the $\varphi$-type of a node is exponential. This gives the path index bound.

Theorem 1 follows from combining Lemma 1 with the following result on satisfiability of NavXP:

**Theorem 2.** The satisfiability of a NavXP filter $\varphi$ over trees of bounded depth $b$ is in PSPACE (in $b$ and $|\varphi|$).

The result is proved in the appendix, but it is a variant of a result from [BFG08] that finite satisfiability for the fragment of NavXP which contains only axis relations child, parent, next-sibling, preceding-sibling, previous-sibling and following-sibling is in PSPACE. Given Theorem 2 we complete the proof of Theorem 1 by translating an FO$^2$ sentence $\varphi$ into a NavXP filter $\varphi'$ with an exponential blow-up, using Proposition 1. By Lemma 1 the depth of a witness structure is bounded by an exponential in $|\varphi|$, and the EXPSPACE result follows.

**Lower bound.** We now show a matching lower bound for the satisfiability problem.

**Theorem 3.** The satisfiability problem for FO$^2$ is EXPSPACE-hard, with hardness holding even when formulas are restricted to be in FO$^2[V_{\text{ancOf}}]$.

This is proved by coding the acceptance problem for an alternating exponential time machine. A tree node can be associated with an $n$-bit address, either by using multiple predicates (for FO$^2[V_{\text{ancOf}}]$) or via children. The equality and successor relations between the addresses associated to nodes $x$ and $y$ can be
coded in \( \text{FO}^2 \) using the standard argument (see the \( \text{NEXPTIME} \)-hardness proof of [EVW02]). A path corresponds to one thread of the alternating computation, and the tree structure is used to code alternation.

4 Satisfiability without child

The exponential depth bound revisited. As noted in the previous section, the satisfiability problem is still \( \text{EXPSPACE} \)-complete even when the ChildOf relation is removed. However, we take a closer look at this case, noting some connections with other logics and some further restrictions that lower the complexity.

We first consider the relationship of \( \text{FO}^2 \) without child to modal tree languages.

Let downward stutter-free \( \text{NavXP} \), denoted \( \text{DownSF-NavXP} \), be the fragment of \( \text{NavXP} \) obtained by restricting to the descendant, ancestor, and all sibling axes. The complexity of satisfiability \( \text{DownSF-NavXP} \) has not been studied in prior work, including [BFG08], but we can show the following depth bound for \( \text{DownSF-NavXP} \):

**Theorem 4.** Every satisfiable \( \text{DownSF-NavXP} \) sentence has a model of polynomial depth. The satisfiability problem for \( \text{DownSF-NavXP} \) is \( \text{PSPACE} \)-complete.

The proof resembles the result that a satisfiable stutter-free temporal logic formula has a model of polynomial size. Some care needs to be taken to deal with the sibling axes, which allow a \( \text{DownSF-NavXP} \) formula to look off of a given path.

This result shows that tight bounds for two-variable logic without child can actually be obtained via translation to modal languages: Combining the first part of Theorem 4 and the translation to \( \text{NavXP} \) from Proposition 1 we get an alternative proof of the exponential depth bound in Lemma 1 as well as the \( \text{EXPSPACE} \) upper bound for satisfiability, in the special case of \( \text{FO}^2[\text{VnoParOf}] \).

**Unary Alphabet Restriction, polynomial alternation bounds, and polynomial depth bounds.** The previous section showed \( \text{EXPSPACE} \)-completeness for satisfiability of \( \text{FO}^2[\text{VancOf}] \). However the \( \text{EXPSPACE} \)-hardness argument for \( \text{VancOf} \) makes use of multiple predicates holding at a given node, to code the address of a tape cell of an alternating \( \text{EXPTIME} \) Turing Machine. It thus does not apply to satisfiability over Unary Alphabet Restriction trees (as defined in Section 2) or to satisfiability with respect to a schema, since schemas restrict to a single alphabet symbol per node. We show that the complexity of satisfiability is actually “lower” (that is, modulo the assumption \( \text{NEXPTIME} \neq \text{EXPSPACE} \)) when the UAR is imposed, using distinct techniques for the case of ranked and unranked trees.

We start by noting that one always has at least \( \text{NEXPTIME} \)-hardness, even with UAR.

**Theorem 5.** The satisfiability of \( \text{FO}^2[\text{VancOf}] \) with the unary alphabet restriction is \( \text{NEXPTIME} \)-hard, and similarly with respect to a ranked schema.

The proof is a variation of the argument for \( \text{NEXPTIME} \) hardness for words [EVW02], but this time using the frontier of a shallow but wide tree to code the tiling of an exponential grid.
We will prove a matching NEXPTIME upper bound for UAR trees and for satisfiability with respect to a ranked schema. To do this, we extend an idea introduced in the thesis of Philipp Weis [Wei11], working in the context of $\text{FO}^2[\prec]$ on UAR words: polynomial bounds on the number of times a formula changes its truth value while keeping the same symbol along a given path.

The following is a generalization of Lemma 2.1.10 of Weis [Wei11].

Consider an $\text{FO}^2[\text{VancOf}]$ formula $\varphi(x)$, a tree $t$ satisfying the UAR, and fix a root-to-leaf path $p = p_1 \cdots p_{\max(p)}$ in $t$. Given a label $a$, define an $a$-interval in $p$ to be a set of the form $\{i : m_1 \leq i < m_2; t, p_i \models a(x)\}$.

**Lemma 3.** For every $\text{FO}^2[\text{VancOf}]$ formula $\varphi(x)$, UAR tree $t$, and root-to-leaf path $p = p_1 \cdots p_{\max(p)}$ in $t$, the set $\{i \mid t, p_i \models \varphi \wedge a(x)\}$ is made up of at most $|\varphi|^2$ $a$-intervals.

From Lemma 3 we will show that $\text{FO}^2[\text{VancOf}]$ sentences that are satisfiable over UAR trees always have polynomial-depth witnesses:

**Lemma 4.** If an $\text{FO}^2[\text{VancOf}]$ formula $\varphi$ is satisfied over a UAR tree, then it is satisfied by a model of depth bounded by a polynomial in $|\varphi|$.

**Proof.** Suppose that $\varphi$ is satisfied over a UAR tree $t$. On each path $p$, for each letter $b$, let a $b, \varphi$-interval be a maximal $b$-interval on which every one-variable subformula of $\varphi$ has constant truth value. By the lemma above, the total number of such intervals is polynomially bounded. We let $W$ contain the endpoints of each $b, \varphi$-interval for all symbols $b$. We note the following crucial property of $W$: for every node $m$ in $p$ which is not in $W$, there is a node in $W$ with the same $\varphi$-type as $m$ that is strictly above $m$, and also one strictly below $m$.

![Fig. 1. Tree Promotion](image)

The idea is now to remove all those points on path $p$ that are not in $W$. This must be done in a slightly unusual way, by “promoting” subtrees that are off the path. For every removed node $r$, for every child $c$ of $r$ not on $p$, we attach the subtree rooted at $c$ to the closest node of $W$ above $r$ (see Figure 1). Let $t'$ denote the tree obtained as a result of this surgery. Formally, the nodes of $t'$ are all nodes of $t$ that are not in $p$ or are in $W$. Each such node has the same label that it had in $t$. For any node $m$ in $t$ with parent $n$, if both $m$ and $n$ are in $t'$
then \( n \) is again the parent of \( m \) in \( t' \). On the other hand, if only \( m \) is in \( t' \) then its parent in \( t' \) is its lowest ancestor in \( W \).

Let \( f \) be the partial function taking a node in \( t \) that is not removed to its image in \( t' \). We claim that \( t' \) still satisfies \( \varphi \), and more generally that for any subformula \( \rho(x) \) of \( \varphi \) and node \( m \) of \( t \), we have \( t, m \models \rho \) iff \( t', f(m) \models \rho \). This is proved by induction on \( \rho \), with the base cases and the cases for boolean operators being straightforward. For an existential formula \( \exists y \beta(x, y) \), we give just the “only if” direction, which is via case analysis on the position of a witness node \( w \) such that \( t, m, w \models \beta \).

If \( w \) is in \( t' \) then \( t', m, w \models \beta \) by the induction hypothesis and the fact that \( w \) is an ancestor (or descendant) of \( m \) in \( t' \) if and only if it is an ancestor (or descendant) of \( m \) in \( t \).

If \( w \) is not in \( t' \), then it must be that \( w \) lies on the path \( p \) and is not one the protected witnesses in \( W \). But then \( w \) has both an ancestor \( w' \) and descendant \( w'' \) in \( W \) that satisfy all the same one-variable subformulas as \( w \) does in \( t \), with both \( w' \) and \( w'' \) preserved in the tree \( t' \). If \( m \) and \( w'' \) are distinct then \( t', m, w'' \models \beta \) by the induction hypothesis and the fact that \( m \) and \( w'' \) have the same ancestor/descendant relationship in \( t' \) as do \( m \) and \( w \) in \( t \). If \( m \) is identical to \( w'' \) then \( t', m, w' \models \beta \) by similar reasoning. In any case we deduce that \( t', m \models \exists y \beta \).

Since this process reduces both the length of the chosen path \( p \) and does not increase the length of any other path, it is clear that iterating it yields a tree of polynomial depth.

Note that we can guess a tree as above in \( \text{NEXPTIME} \), and hence we have the following bound:

**Theorem 6.** Satisfiability for \( \text{FO}^2[\text{VancOf}] \) formulas over UAR unranked trees is in \( \text{NEXPTIME} \), and hence is \( \text{NEXPTIME}\)-complete.

**Bounds on subtrees and satisfiability of \( \text{FO}^2[\text{VancOf}] \) with respect to a ranked schema.** The collapse argument above relied heavily on the fact that trees were unranked, since over a fixed rank we could not apply “pathwise collapse”. Indeed, we can show that over ranked trees, a \( \text{FO}^2[\text{VancOf}] \) formula satisfiable over UAR trees need not have a witness of polynomial depth:

**Theorem 7.** There are \( \text{FO}^2[\text{VancOf}] \) formulas \( \varphi_n \) of size \( O(n) \) that are satisfiable over UAR binary trees, where the minimum depth of satisfying UAR binary trees grows as \( 2^n \).

Nevertheless, we can still obtain an \( \text{NEXPTIME} \) bound for UAR trees of a given rank, and even for satisfiability with respect to a ranked schema.

**Theorem 8.** The satisfiability problem for \( \text{FO}^2[\text{VancOf}] \) over ranked schemas is in \( \text{NEXPTIME} \), and is thus \( \text{NEXPTIME}\)-complete.

We give the argument only for satisfiability with respect to rank-\( k \) UAR trees, leaving the extension to schemas for the appendix. This will also serve as an alternative proof of Theorem 6. The idea will be to create a model with only an exponential number of distinct subtrees, which can be represented by
an exponential-sized DAG. We do this by creating an equivalence relation that is 
globally ϕ-preserving (not just pathwise) and which has exponential index (not 
just path index). We will then collapse equivalent nodes, as in Lemma 2. There 
are several distinctions from that lemma: to identify nodes that are not necessarily 
comparable we can not afford to abstract a node by the set of all the types realized 
below it, since within the tree as a whole there can be doubly-exponentially many 
such sets. Instead we will make use of some “global information” about the tree, 
in the form of a set of “protected witnesses”, which we denote W.

By Lemma 1 we know that a satisfiable FO²[V\text{anc}_O] formula ϕ has a model 
t of depth at most exponential in ϕ. Fix such a t. For each ϕ-type τ, let wτ be a node of t with maximal depth satisfying τ. We include all wτ and all of 
their ancestors in a set W, and call these basic global witnesses. For any m 
that is an ancestor or equal to a basic global witness wτ, and any subformula ρ(x) = ∃yβ(x,y) of ϕ, if there is w′ incomparable (by the descendant relation) to 
m such that t,m,w′ |= ϕ we add one such w′ to W, along with all its ancestors – 
these are the incomparable global witnesses.

We need one more definition. Given a node m in a tree, for every ϕ-type τ realized by some ancestor m′ of m, for every subformula ∃yβ(x,y) of τ, if 
there is a descendant w of m such that t,m,w |= β we add one such W to W, 
along with all its ancestors – these are the selected global witnesses.

Now we transform t to t′ such that t′ |= ϕ and t′ has only exponentially 
many different subtrees. We make use of a well-founded linear order ≺ on trees with a given rank and label alphabet, such that: 1. SubTree(t,n′) ≺ SubTree(t,n) 
implies n′ is not an ancestor of n; 2. for every tree C with a distinguished leaf, for tree t1,t2 with t1 ≺ t2, we have C[t1] ≺ C[t2], where C[t_i] is the tree obtained by 
replacing the distinguished leaf of C with t_i. There are many such orderings, 
e.g. using standard string encodings of a tree.

For any model t if there are two nodes n,n′ in t such that 1. n,n′ ∉ W, 
2. Tp_n(n) = Tp_n(n′), 3. AncTypes(n) = AncTypes(n′), 4. SelectedDescTypes(n) 
= SelectedDescTypes(n′), 5. SubTree(t,n′) ≺ SubTree(t,n) (which implies that 
n′ cannot be an ancestor of n), then let t′ = Update(t) be obtained by choosing such n and n′ and replacing the subtree rooted at n by the subtree rooted at n′.

Let T_1 be the nodes in t that were not in SubTree(t,n), and for any node 
m \in T_1 let f(m) denote the same node considered within t′. Let T_2 denote the nodes in t′ that are images of a node in SubTree(t,n′). For each m \in T_2, let f^{-1}(m) denote the node in SubTree(t,n′) from which it derives.

We claim the following:

**Lemma 5.** For all m \in T_1 the ϕ-type of n in t is the same as the ϕ-type of 
f(m) in t′. Moreover, for every node m′ in T_2, the ϕ-type of m′ in t′ is the same 
as that of f^{-1}(m) in t.

Applying the lemma above to the root of t, which is necessarily in T_1, it 
follows that the truth of the sentence ϕ is preserved by this operation.
We now iterate the procedure \( t_{i+1} := \text{Update}(t_i) \), until no more updates are possible. This procedure terminates, because the tree decreases in the order \( \prec \) every step. We can thus represent the tree as an exponential-sized DAG, with one node for each subtree.

Thus we have shown that any satisfiable formula has an exponential-size DAG that unfolds into a model of the formula. Given such a DAG, we can check whether an FO\(^2\) formula holds in polynomial time in the size of the DAG. This gives a NEXPTIME algorithm for checking satisfiability.

5 Satisfiability without descendant

Recall that even on words with only the successor relation, the satisfiability problem for two-variable logic is NEXPTIME-hard [EVW02]. From this it is easy to see that the satisfiability for FO\(^2\)[\(V_{parOf}\)] is NEXPTIME-hard, on ranked and unranked trees.

**Theorem 9.** The satisfiability problem for FO\(^2\)[\(V_{parOf}\)] is NEXPTIME-hard, even with the unary alphabet restriction.

We now present a matching upper bound, which holds even in the presence of sibling relations, i.e., for FO\(^2\)[\(V_{noAncOf}\)]. The result is surprising, in that it is easy to write satisfiable FO\(^2\)[\(V_{parOf}\)] sentences \( \varphi_n \) of polynomial size whose smallest tree model is of depth exponential in \( n \), and whose size is doubly exponential. Indeed, such formulas can be obtained as a variation of the proof of Theorem 9, by coding a complete binary tree whose nodes are associated with \( n \)-bit numbers, increasing the number by 1 as we move from parent to either child.

The result below relies on the fact that one can witness the satisfiability of a given formula by an exponential-sized DAG.

**Theorem 10.** The satisfiability problem for FO\(^2\)[\(V_{noAncOf}\)], and the satisfiability problem with respect to a rank schema, are in NEXPTIME, and hence are NEXPTIME-complete.

We sketch the idea for satisfiability, which iteratively quotients the structure by an equivalence relation, while preserving certain global witnesses, along the lines of Theorem 8. By Lemma 1 we know that a satisfiable FO\(^2\)[\(V_{noAncOf}\)] formula \( \varphi \) has a model \( t \) of depth at most exponential in \( \varphi \), where the outdegree of nodes is bounded by an exponential.

For each \( \varphi \)-type that is satisfied in \( t \), choose a witness and include it along with all its ancestors in a set \( W \) – that is, we include the “basic witnesses” as in Theorem 8. We also include all children of each basic witness – call these “child witnesses”.

Thus the size of the set of “protected witnesses” \( W \) is again at most exponential. Now we transform \( t \) to \( t' \) such that \( t' \models \varphi \) and at the same time \( t' \) has only exponentially many different subtrees. Our update procedure looks for nodes \( n, n' \) in \( t \) such that 1. \( n, n' \notin W \); 2. \( \text{SubTree}(t, n') \prec \text{SubTree}(t, n) \), where \( \prec \) is an appropriate ordering (as in Theorem 8); 3. \( T_\varphi(n) = T_\varphi(n') \) and \( T_\varphi(\text{parent}(n)) = T_\varphi(\text{parent}(n')) \). We then obtain \( t' = \text{Update}(t) \) by choosing such \( n \) and \( n' \) and replacing \( \text{SubTree}(t, n) \) by \( \text{SubTree}(t, n') \).
The theorem is proved by showing that this update operation preserves $\varphi$. Iterating it until no two nodes can be found produces a tree that can be represented as an exponential-size DAG.

6 Conclusions

We have shown that the parallel between the complexity of $\text{FO}^2$ satisfiability on general structures and on restricted structures breaks down as we move from words to trees – trees allow one to encode alternating exponential time computation, leading to $\text{EXPSPACE}$-hardness. On the other hand, we show that analogs of the “model shrinking” methods for $\text{FO}^2$ on words exist for trees, albeit using a different shrinking technique. In future work, we are extending the analysis to infinite trees, where we believe it can be useful for analyzing branching time properties of both non-deterministic and probabilistic systems, as was done for linear time in [BLW12]. We are also considering the case of structures of fixed tree-width.

Our main complexity results on satisfiability are summarized in Table [6] where in each case the bound is tight.

|           | $\text{FO}^2$ | $\text{FO}^2[\text{ancOf}]$ | $\text{FO}^2[\text{noParOf}]$ | $\text{FO}^2[\text{parOf}]$ |
|-----------|---------------|-----------------|-----------------|-----------------|
| All Trees | $\text{EXPSPACE}$ | $\text{EXPSPACE}$ | $\text{EXPSPACE}$ | $\text{NEXPTIME}$ |
| w.r.t. Ranked Schema | $\text{EXPSPACE}$ | $\text{NEXPTIME}$ | $\text{EXPSPACE}$ | $\text{NEXPTIME}$ |

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More detail on the proof of Lemma \(\text{1}\) and Lemma \(\text{2}\)

We first give a detailed proof of the following statement from Lemma \(\text{2}\):

The equivalence relation \(\equiv_{\text{full}}\) is pathwise \(\varphi\)-preserving.

Fix tree \(t\) and \(n_0 \equiv_{\text{full}} n_1\) lying on the same path \(p\) in \(t\), with \(n_1\) a descendant of \(n_0\). Let \(t'\) be formed by overwriting \(n_0\) with \(n_1\), and \(f\) be the mapping taking a node that lies in the subtree of \(n_1\) or outside of the subtree of \(n_0\) to its image in \(t'\). By the “collapsed part of \(t'\)” we refer to the part of \(t\) not in the domain of \(f\).

We prove via structural induction that for every subformula \(\rho\) of \(\varphi\) and node \(m\) in the domain of \(f\) we have \(t, m \models \rho \iff t', f(m) \models \rho\). The atomic cases and the boolean operators are clear, so existential quantification is the only non-trivial case.

Consider first a node \(m\) in the bottom half of the non-collapsed structure – that is, in \(\text{SubTree}(t, n_1)\) – satisfying \(\rho(x) = \exists y \beta(x, y)\). By induction we need consider only the case where some node \(w\) witnessing that \(m\) satisfies \(\rho\) in \(t\) is not in the domain of \(f\). Fix such a witness node \(w\). We show that we can find a node that satisfies the same one-variable subformulas of \(\rho\) that \(w\) does, and which satisfies the same axis relations with respect to \(m\) that \(w\) does.

When the witness to the existential quantifier in \(\rho\) is a parent of \(m\), then we must have \(m = n_1\). Now we can apply the hypothesis that the \(\varphi\)-type of \(n_0\) is the same as the \(\varphi\)-type of \(n_1\), plus the induction hypothesis, to conclude that \(f(m)\) must satisfy \(\rho\). The case in which the witness \(w\) is a descendant of \(m\) or equal to \(m\) need not be considered, since such a witness must be in the domain of \(f\), which is ruled out by assumption. Now consider the case where some witness \(w\) is an ancestor of \(m\), but not a parent. Such a \(w\) must be on the path \(p\). In this case, we can use the fact that \(\text{AncTypes}(n_0) = \text{AncTypes}(n_1)\) to argue that a witness can be found. Suppose there is a node \(w\) witnessing that \(t, m \models \rho(x)\) such that \(w\) is not an ancestor or a descendant of \(m\). Then we can apply the fact that \(\text{IncompTypes}(n_0) = \text{IncompTypes}(n_1)\) to find a witness \(w'\) that is incomparable of \(n_0\), but still in the domain of \(f\). Such a \(w\) can be used (by induction) as a witness that \(t', f(m) \models \rho\).

We now move to the case where \(m\) is in the top half of the non-collapsed structure satisfying \(\rho(x) = \exists y \beta(x, y)\). We are interested in the case where all witnesses \(w\) to the existential quantifier in \(\rho\) are in the collapsed part of the structure, and hence are not ancestors of \(m\).

Suppose we have a witness that is not a descendant or ancestor of \(m\). The witness must be a descendant of \(n_0\), and \(n_0\) must not be a descendant of \(m\). We can apply again the fact that \(\text{DescTypes}(n_0) = \text{DescTypes}(n_1)\) to find a witness \(w'\) below \(n_1\), which will suffice by induction.

If the witness \(w\) is in the collapsed part of \(t\) and is a child of \(m\), we must have \(m = n_0\), and hence we can use the fact that \(\text{Tp}_\varphi(n_0) = \text{Tp}_\varphi(n_1)\) to get the desired witnessed. Now suppose we have a witness \(w\) in the collapsed part of the structure, with \(w\) a descendant of \(m\) but not a child of \(m\). Again, if \(m = n_0\) we are done, using the fact that \(\text{Tp}_\varphi(n_0) = \text{Tp}_\varphi(n_1)\). If \(m \neq n_0\), we must have \(m\) is a strict ancestor of \(n_0\). From \(\text{DescTypes}(n_0) = \text{DescTypes}(n_1)\) we know that
there is a descendant $w'$ of $n_1$ with the same $\varphi$-type as $w$. Since $m \neq n_0$ $w'$ is not a child of $m$ in $t'$, and hence can serve as a witness.

The cases for the sibling axes are also straightforward, since no nodes in the domain of $f$ have their siblings modified by the collapse mapping.

We now explain the variation of the argument for the exponential bound on branching. Note that NavXP queries can already force exponential branching, and thus the result does not follow directly via translation to modal tree logics. In a nutshell, we use the same approach, but shrinking horizontal rather than vertical paths.

**Construction**: Consider the equivalence relation that relates two nodes if they have:

- the same $\varphi$-types that occur as left-siblings, and the same $\varphi$-types that occur as right-siblings
- the same $\varphi$-types of nodes that are descendants of right-siblings, and similarly for left-siblings
- the same $\varphi$-types, and the same $\varphi$-types immediately to the right and immediately to the left

Recall that the right-sibling relation is the transitive closure of the immediate right-sibling relation, and similarly for left-sibling. Note that the first two items change only exponentially many times, and on an interval where they are both constant, the third item takes on only exponentially many values.

We now claim that any sufficiently long horizontal path can be pruned. Fix a horizontal path $p$ containing all children of some node. If $p$ is sufficiently long, there is some equivalence class $C$ that has more than one node in it. Let $n'$ be the left-most (lowest in sibling order) element of $C$, and $n$ the element of $C$ that is closest to it on the right. Let $t'$ be obtained by removing all subtrees of nodes between $n'$ and $n$, including the subtree of $n$ but not the subtree of $n'$.

**Correctness**: Let $f$ be the function taking a node in $t$ that was not removed by the operation above (for short “non-removed node”) to its image in $t'$. As usual, we proceed by showing that $\varphi$-types are preserved in moving from a node $m$ to $f(m)$. As before, the only important case is the inductive step for $\rho(x) = \exists y \beta(x, y)$, with the non-trivial direction being to show that if $\rho$ holds at $t, m$ then it holds in $t', f(m)$. Suppose $m$ satisfies $\rho$, with witness $w$. The interesting case is when $w$ is a removed node, which means it must either be a right-sibling of $n'$ that was removed or below a right-sibling of $n'$ that was removed. We do case analysis on the relationship of $w$ to $m$.

**Case of Incomparable Witnesses**: If $w$ is incomparable to $m$ by both the sibling and ancestor relations, then we consider several subcases.

The first subcase is where $m$ is “below a node in $p$” – that is, a descendant of some node on $p$. Let $n''$ be the node of $p$ that is an ancestor of $m$.

We further consider the subsubcase where the sibling $n''$ is to the right of $n$. If $w$ is a right-sibling of $n'$, then it was a left-sibling of $n$ or is equal to $n$, since these are the siblings that are removed. In the first case, it must be that $n'$ has a left-sibling $w'$ with the same $\varphi$-type as $w$. Since $m$ is “down and to the right”
(that is, below a right-sibling) of \( n' \), \( w' \) is incomparable to \( m \), and thus such a \( w' \) can be used as a witness that \( t', f(m) \models \rho \). Similarly, in the case that \( w \) was equal to \( n \), \( n' \) can be used as a witness. If \( w \) is below a right-sibling of \( n' \), it must be that \( n' \) has a left-sibling that has a descendant with the same \( \varphi \)-type, and this can be used as a witness.

The paragraph above completes the subsubcase where \( n'' \) is to the right of \( n \). If \( n'' \) is to the left of, or is equal to, \( n' \), we argue symmetrically, but considering the \( \varphi \)-types that are right-siblings or descendants of right-siblings of \( n \).

The subcase where \( m \) is itself a sibling of \( n \) is similar to the above, except \( w \) cannot be a sibling of \( m \), and hence one subcase does not need to be considered.

The final subcase is where \( m \) is not on \( p \) and is not a descendant of a node in \( p \). Note the assumption that \( w \) is incomparable to \( m \) and removed during the collapse process, and hence \( w \) lies below a node on the horizontal path \( p \). This implies that \( m \) can not be an ancestor of the nodes in \( p \). If \( w \) is a sibling of a node in \( p \) that was removed, we can use any non-removed sibling of \( n' \) with the same \( \varphi \)-type as a witness (there are at least two such nodes, to the left and right). Similarly if \( w \) is below a sibling of a removed node of \( p \), we use any non-removed node that has the \( \varphi \)-type of \( w \) and which is a descendant of a node on \( p \).

**Other cases:** The case where the witness \( w \) is a descendant of \( m \) is similar to the last subcase above. In this case, \( m \) must be an ancestor of the nodes on \( p \). Again, if \( w \) is a sibling of \( n \), we can choose a sibling with the same \( \varphi \)-type. If \( w \) is a descendant of a sibling, we can choose a descendant of a sibling with the same \( \varphi \)-type.

We now turn to the case where \( w \) is an immediate left-sibling of \( m \). In this case we must have \( m = n \), and we can use the fact that \( n \) and \( n' \) have the same \( \varphi \)-type for their immediate left-siblings. The case where \( w \) is an immediate right-sibling of \( m \) is analogous.

The case where \( w \) is a following-sibling but not the next-sibling, or a preceding-sibling but not the previous-sibling, is handled similarly to above.

Iterating this pruning process gives the required branching bound.

**Proof of Theorem 2**

Recall the statement:

*The satisfiability of a NavXP filter \( \varphi \) over trees of bounded depth \( b \) is in PSPACE (in \( b \) and \( |\varphi| \)).*

It can be awkward to work with NavXP, since one has to switch back between two- and one-variable formulae. For simplicity, we work with a temporal logic \( UTL_{tree} \) for trees analogous to Unary Temporal Logic on words, introduced in [LS08]. Formulas \( \varphi \) are given by:

\[
\varphi ::= \varphi_1 \mid \varphi_1 \land \varphi_2 \mid \neg \varphi_1 \mid \Diamond_1 \varphi_1 \mid \Diamond_{\varphi_1} \mid \Box_{\varphi_1} \mid \Box_1 \varphi_1
\]

where \( * \) stands for either a child (CH) relation or a next-sibling relation (NS). Informally \( \Diamond_{CH} \varphi \) is “eventually along a vertical path \( \varphi \) holds”, \( \Diamond_{CH} \) is “up the vertical path to the root”, \( \Box_{CH} \) is “in some child” and \( \Box_{CH} \) “in the parent”. The variants for NS are defined similarly for horizontal paths. The semantics of \( UTL_{tree} \) with respect to a tree \( T \) and node \( s \) is given as a variant
of the standard semantics for linear temporal logic on words. For example
\((T, s) \models P_i \iff s \text{ has label } P_i\). The boolean operators have their usual recursive
definition. \((T, s) \models \Box_{CH} \varphi \iff \exists s' \text{ such that } s' \text{ ChildOf } s \text{ and } (T, s') \models \varphi\),
and similarly for the other next state modalities.

The above semantics maps a formula to a set of nodes in a tree. For a tree \(t\),
we say \(t \models \varphi\) to mean \((t, n_0) \models \varphi\) where \(n_0\) is the root.

[LS08] shows that \(\text{NavXP}\) can be translated in polynomial time into \(UTL_{\text{tree}}\).

We give a non-deterministic \(\text{PSPACE}\) algorithm that constructs a witness tree
for \(\varphi\), materializing only the rightmost branch of the tree. As an abstraction of
this branch the algorithm guesses all the \(\varphi\)-types of nodes appearing on the path
to the root, along with auxiliary information about whether a node is the last
child of its parent, and which subformulas of the form \(\Box_{CH} \psi\) and \(\Diamond_{CH} \psi\) have
been satisfied.

We require all guessed types to be internally consistent, and to satisfy certain
consistency properties. Additionally, we require \(\varphi\) to be in the type of the root.

Now we show how to check the consistency for all temporal subformulas.

1. Subformulas \(\Box_{CH} \psi\) and \(\Diamond_{CH} \psi\) are the easiest to check, because for each node
we have already guessed all its ancestors.

2. When we extend a path downward (corresponding to guessing the type of
the initial child), we require that all subformulas \(\Box_{NS} \psi\) are false and that
the truth value of \(\Diamond_{NS} \psi\) is equivalent to truth value of \(\psi\). When we move
from a leaf \(l\) of a path to its sibling, we enforce that the new type contains
\(\Diamond_{NS} \psi\) if \(l\) contains it, and that it contains \(\Box_{NS} \psi\) iff \(l\) contains \(\psi\).

3. When we move to a sibling of \(l\), if \(l\) contains \(\Box_{NS} \psi\), we ensure that the type
of the newly-created sibling contains \(\psi\). For \(\Box_{NS} \psi\), we guess that its sibling
contains \(\psi\) or \(\Diamond_{NS} \psi\). If we guess that a leaf is the rightmost sibling, we check
that its type does not contain \(\Diamond_{NS} \psi\).

4. For subformulas \(\Box_{CH} \psi\) and \(\Diamond_{CH} \psi\), we mark whether they have already been
satisfied by some prior descendant. If not, we decide when we extend the
path whether or not they will be satisfied on the new child, and guess the
type accordingly. When we move from a leaf \(l\) to its sibling, we require that
every such formula that was in \(l\) has been marked as satisfied.

Proof of Theorem 3
Recall the statement:

The satisfiability problem for \(\text{FO}^2\) is \(\text{EXPSPACE}\)-hard, and the same holds for
\(\text{FO}^2[\text{ancOf}]\).

We first give the argument for \(\text{FO}^2\). We reduce from the problem of determining
whether an alternating \(\text{EXPTIME}\) Turing Machine \(T\) accepts a given input \(I\).
Without loss of generality we assume that each configuration of \(T\) has exactly
two successors. We can also assume that for an input of size \(n\), the computation
of \(T\) takes at most \(2^n\) steps and therefore uses at most \(2^n\) tape cells. We give a
polynomial time transformation that takes \(T\) and machine input \(I\), returning an
\(\text{FO}^2\) formula \(\varphi\) which is satisfiable if and only if \(T\) accepts \(I\).

We encode each tape configuration as a sequence of \(2^n\) nodes with one node
per cell. Each cell will have a label encoding:
– the tape symbol written on the cell
– the time step (or “index”) of the configuration, encoded in \( n \) bits \( c_1, c_2, \ldots, c_n \)
– the cell position encoded in \( n \) bits \( p_1, p_2, \ldots, p_n \)
– the control state of the Turing Machine
– the last alternation choice, which is either \( \land \) or \( \lor \)
– whether the head of the Turing Machine is present

The computation of \( T \) will be described by a tree of tape computations starting with an initial configuration. Intuitively the formula \( \varphi \) will force the shape of the tree to match that of the computation tree for \( T \). In more detail, an \( \land \)-configuration will be represented in the tree by a path of \( 2^n \) nodes that terminates in a node with two children, each of which is the root of a successor configuration. On the other hand an \( \lor \)-configuration is represented by a path of \( 2^n \) nodes that terminates in a node with a single child, which is the root of a single successor configuration. The vocabulary of the formula will have predicates for the presence or absence of the Turing machine head, the alternation choice, the tape alphabet symbols, and predicates indicating which of \( c_1, \ldots, c_n, p_1, \ldots, p_n \) hold.

Now we discuss in more detail the parts of \( \varphi \) that will ensure the structure described above. The tree should have as root a node whose index is a vector of zeros for the values of \( c_1, \ldots, c_n, p_1, \ldots, p_n \), after which we need to increase the number represented by this vector by one for each child node. Within the same configuration the latter can be easily enforced by the following formula:

\[
\forall x \forall y \left( \text{ChildOf } x \rightarrow \bigvee_i \left( \neg p_i(x) \land p_i(y) \land \bigwedge_{j<i} p_j(x) \leftrightarrow p_j(y) \land \bigwedge_{j>i} p_j(x) \land \neg p_j(y) \right) \right)
\]

We can use the predicates \( c_i \) and \( p_i \) (and formulas similar to the one above) to determine whether two nodes \( x \) and \( y \) corresponding to tape cells in a configuration of \( T \) represent the same, previous or next position within the same configuration, or whether they are in the same, previous, or next configuration. For example, two nodes that represent successive configurations in a single thread of a machine will need to be in the \( \text{DescOf} \) relation, and will have configuration co-ordinates that are in a successor relation, which will be enforced as above, but using the \( c_i \) rather than the \( p_i \).

To encode the alternation, we need to enforce that the shape of a node is consistent with the type of the current configuration, in terms of whether the state is universal or existential. For example, if we have a universal state \( q \) and a transition to control states \( q_1 \) and \( q_2 \), after the last cell of the configuration we will enforce that there is a child whose control state is \( q_1 \) and another child whose control state is \( q_2 \).

We have a formula \( \psi(x, y) \) that checks the consistency of the tape cells represented by nodes \( x \) and \( y \) that are in a descendant relationship (and hence represent the same thread in the alternating computation). If \( x \) and \( y \) point to the same cell position in consecutive configurations then we need the content of \( x, y \) and their adjacent cells to be consistent with the transition function of \( T \),
the position of the head, the current state, the cell symbols and the alternation type (\(\land vs \lor\)).

The enforcement that the input is on the tape initially, and that an acceptance state is reached at each leaf, can similarly be easily enforced.

**Extension of the argument from** \(\text{FO}^2\) **to** \(\text{FO}^2[\text{V}_{\text{parOf}}]\).** In the proof above we use only the \text{DescOf} and \text{ChildOf} relations. We now show how to avoid \text{ChildOf}. The key is that we do not need consecutive positions within the same configuration to occur in a parent child relationship. Along any thread, we can uniquely identify via the predicates \(c_1 \ldots c_n\) and \(p_1 \ldots p_n\). We can thus consider nodes correspond to consecutive positions in the same configuration using these predicates, while using \text{DescOf} to restrict to nodes within the same thread.

We will enforce that

- each descendant of any node has a larger configuration index
- each node (except the first) has an ancestor whose configuration address is smaller by one
- each node is either a representative of the last configuration in its thread (i.e. with maximal configuration index) or it has a descendant whose configuration index is higher by one

We have similar requirements for the position indices for the same configuration.

**Proof of Theorem 4**

Recall the key statement:

*Every satisfiable \text{DownSF-NavXP} sentence has a model of polynomial depth.*

Again, since it is more convenient to deal with one-variable formula than a mix of two- and one-variable as in \text{NavXP}, we will prove this for the modal tree logic formed from \(\text{UTL}_{\text{tree}}\) by removing the child and parent modalities (but including the next- and previous- sibling modalities). Call the resulting language \(\text{TL}_{\text{tree}}\).

Consider a satisfiable \(\text{TL}_{\text{tree}}\) formula \(\varphi\), a tree \(t\) satisfying \(\varphi\), and a path \(p\) in \(t\). We will shrink \(p\) to polynomial size without impacting \(\varphi\), and iterating this process we can achieve polynomial depth. Once we achieve polynomial depth, we can use Theorem 2 to get a \(\text{PSPACE}\) bound.

The **vertical \(\varphi\)-type** of \(n\) is defined as the collection of subformulas of \(\varphi\) of the form \(\bigodot_{\text{CH}}\psi\) or \(\bigotimes_{\text{CH}}\psi\) that hold at \(n\), along with the formula \(a(x)\) where \(a\) is the label of \(n\).

The following lemma generalizes an obvious fact about the usual stutter-free temporal logic on words:

**Lemma 6.** There are polynomially many (in \(|\varphi|\)) vertical \(\varphi\) type changes along any path \(p\).

*Proof.* Consider a path \(p\) of \(T\) and a node \(n\) of \(p\). If \(n \not\models \bigodot_{\text{CH}}\psi\), then in all subsequent nodes \(n'\) in the path, \(n' \not\models \bigodot_{\text{CH}}\psi\). Similarly if \(n \not\models \bigotimes_{\text{CH}}\psi\), then in all previous nodes \(n'\) in the path, \(n' \not\models \bigotimes_{\text{CH}}\psi\). We therefore have that these subformulas change their truth assignment at most once in \(p\).
We are now ready to prove the polynomial depth bound. Consider any (downward) path \( p \) in the tree. By Lemma 6, there are polynomially many vertical type changes along a path.

Consider a maximal interval of \( p \) all of whose nodes have the same vertical type, and let \( n_{\text{High}} \) and \( n_{\text{Low}} \) be the first (highest) and last (lowest) nodes of the interval. Now consider the tree \( t' = t(n_{\text{Low}} \to n_{\text{High}}) \) constructed by overwriting \( n_{\text{High}} \) with \( n_{\text{Low}} \).

Let \( f \) be the partial function taking nodes in \( t \) that are not removed to their images in \( t' \).

As with all of our collapse operations, our goal is to show:

**Claim.** For any subformula \( \rho \) of \( \phi \) and node \( m \) in the domain of \( f \), we have that \( t, m \models \rho \iff t', f(m) \models \rho \).

Thus performing this operation on every interval shrinks \( p \) without impacting \( \phi \), and iterating over all \( p \) gives the depth bound. We prove this by induction on \( \rho \). Atomic propositions and boolean combinations are immediate.

We begin by considering \( \rho = \Diamond_{\text{CH}} \psi \). If \( t, m \models \rho \) then there is a node \( w \) below \( m \) satisfying \( \phi \) in \( t \). If \( w \) is in the domain of \( f \), we are done by induction, so assume \( w \) is a descendant of \( m \) that is not in the domain of \( f \). Thus \( w \) is also a descendant of \( n_{\text{High}} \). Since \( n_{\text{High}} \) has the same downward-type as \( n_{\text{Low}} \), \( n_{\text{Low}} \) has a descendant satisfying \( \rho \), and this can be used as a witness. In the other direction, assume \( t', f(m) \models \rho \). There must therefore be a path of nodes in \( t \) starting with \( m \) leading to a node \( w' \) where \( \psi \) holds, and \( w' \) must be of the form \( f(w) \) for \( w \) in \( t \). By induction \( w \) can be used as a witness that \( t, m \models \rho \). A similar argument holds for \( \rho = \Diamond_{\text{NS}} \psi \).

Note that the sibling nodes of a given node \( m \) in the domain of \( f \) are not impacted by the overwrite operation. Using this it is easy to see that the induction cases for the sibling axes (e.g. \( \rho = \Diamond_{\text{NS}} \psi \)) go through.

This completes the proof of the claim. Iterating the claim gives the proof of the first part of the theorem.

**Proof of Theorem 5**

Recall the statement:

*The satisfiability of \( \text{FO}^2[V_{\text{ancOf}}] \) with the unary alphabet restriction is \( \text{NEXPTIME-hard} \).*

**Proof.** We make use of a standard \( \text{NEXPTIME} \)-complete problem, tiling an exponential sized grid [Bon97].

The input consists of a number \( n \) (in unary), a set \( C = \{1, \ldots, k\} \) of colours, and a vertical and horizontal constraint \( V, H \subset C \times C \). A tiling is a mapping \( f : \{1, 2, \ldots, 2^n\} \times \{1, 2, \ldots, 2^n\} \to C \), and a solution to the tiling problem consists of a tiling such that the vertical and horizontal constraints are satisfied.

Our formula will have in its signature predicates

\[
\text{ZeroX}_1, \text{OneX}_1, \ldots, \text{ZeroX}_n, \text{OneX}_n, \text{ZeroY}_1, \text{OneY}_1, \ldots, \text{ZeroY}_n, \text{OneY}_n
\]

representing bits in the binary representation of the \( x \) - and \( y \)-coordinates of a grid position, along with predicates \( C_1 \ldots C_k \) for the colours, and finally a predicate \( r \)
for the root. We code a tiling \( f \) by a tree consisting of branches of depth \( 2n + 2 \) for each grid position \( \{1, 2, \ldots, 2^n\} \times \{1, 2, \ldots, 2^n\} \). If \( f(x, y) = c \) then the branch will consist of a root, followed by \( n \) nodes, where the \( i \)th is labelled with \( \text{ZeroX}_i \) if the \( i \)th bit of \( x \) is 0 and is labelled with \( \text{OneX}_i \) otherwise. The branch will then have \( n \) nodes coding the \( y \)-coordinate, labelled with \( \text{ZeroY}_i \) or \( \text{OneY}_i \), and finally a leaf labelled with \( c \). Our \( \text{FO}^2[\text{V}_{\text{ancOf}}] \) formula \( \varphi \) will describe the encoding of a valid \( T \)-tiling \( f \). It will include conjuncts enforcing the shape above:

- There is a node with no ancestors labelled \( r \), and this node has a descendant labelled \( \text{ZeroX}_1 \) and another descendant labelled \( \text{OneX}_1 \).
- Any node with label \( \text{ZeroX}_i \) or \( \text{OneX}_i \) for \( i < n \) has a descendant labelled with \( \text{ZeroX}_{i+1} \) and another with \( \text{OneX}_{i+1} \), such a node has no descendants labelled with \( \text{ZeroX}_j, \text{OneX}_j \) for \( j < i \).
- Any node with label \( \text{ZeroX}_n \) or \( \text{OneX}_n \) has descendants labelled with \( \text{ZeroY}_1 \) and another with \( \text{OneY}_1 \), and has no descendants labelled with labels other than \( c \).
- Any node with label \( \text{ZeroY}_i \) or \( \text{OneY}_i \) for \( i < n \) has descendants labelled with \( \text{ZeroY}_{i+1} \) and another with \( \text{OneY}_{i+1} \), and all its descendants are labelled with \( \text{ZeroX}_j, \text{OneX}_j \) for \( j \geq i \) or with \( c \in C \).
- For any node with label \( \text{ZeroY}_n \) or \( \text{OneY}_n \), there is some \( c \in C \) such that \( n \) has a descendant labelled \( c \) and no descendants with labels other than \( c \).
- Nodes labelled with \( c \in C \) are leaves.

One can then write a formula \( \text{SAME-X}(x, y) \) that checks whether two leaf nodes have the same \( x \)-coordinate:

\[
\text{SAME-X}(x, y) = \bigwedge_i ( (\exists y \text{ AncOf } x \wedge \text{ZeroX}_i(y)) \leftrightarrow (\exists x \text{ AncOf } y \wedge \text{ZeroX}_i(x)) )
\]

In the same way we can define \( \text{SAME-Y}(x, y) \) to check whether two nodes agree on their \( y \)-coordinate, and \( \text{PLUS-X}(x, y) \), \( \text{PLUS-Y}(x, y) \) to check whether two nodes represent consecutive \( x \)- and \( y \)-coordinates, respectively.

The formulas above still allow the possibility of many branches with the same co-ordinates but different colors, but this can be enforced by the following formula, where \( \text{LEAF}(x) \) states that \( x \) is a leaf:

\[
\forall x \forall y (\text{LEAF}(x) \wedge \text{LEAF}(y) \wedge \text{SAME-X}(x, y) \wedge c(x)) \rightarrow c(y)
\]

The vertical and horizontal constraints can be enforced in the usual way given the formulas described above. For example:

\[
\forall x \forall y (\text{LEAF}(x) \wedge \text{LEAF}(y) \wedge \text{SAME-X}(x, y) \wedge \text{PLUS-Y}(x, y) \wedge c(x)) \rightarrow \bigvee_{(c, c') \in V} c'(y)
\]

Conjoining these sentences gives an \( \text{FO}^2[\text{V}_{\text{ancOf}}] \) sentence that holds on UAR trees iff a tiling exists.

**Proof of the polynomial alternation bound (Lemma 3)**

Recall the statement of Lemma 3.
Consider an $\text{FO}^2[\text{V}_{\text{ancOf}}]$ formula $\psi$ over unary predicates in $\Sigma$, and a tree $t$ satisfying the UAR. For any symbol $a \in t$, and any root-to-leaf path $p = p_1 \ldots p_{\max(p)}$ in $t$, the set $p(\psi, a) := \{ i \mid t, p_i \models \psi & a(x) \}$ is made up of at most $|\psi|^2$ a-intervals (i.e., intervals in the set $\{ i \mid t, p_i \models a(x) \}$).

The result relies on the following combinatorial lemma, which is adapted from the argument in Lemma 2.1.10 of Weis [Wei11]. Analogously to the terminology above, given a word $w = w_1 \ldots w_{\max(w)}$ and a symbol $a$, by an $a$-interval we mean an interval in the set of positions in $w$ that have label $a$.

**Lemma 7.** Consider a word $w$, a symbol $a$, formulas $\varphi_i(x) : i \leq r$, and $L, U$ functions that assign each boolean valuation of the $\varphi_i(x)$ to positions of $w$. Let $\beta$ be a positive boolean combination in propositions $P_1 \ldots P_j$ and consider the set

$$J(w) := \{ j \in w \mid w(j) = a \wedge (w, j) \models \beta(\varphi_1, \ldots, \varphi_r) \wedge (j \geq L(\text{Val}(j)) \vee j < U(\text{Val}(j))) \}$$

where $\text{Val}(j)$ is the boolean valuation of $\varphi_i : i \leq r$ induced by $j$ in $w$. Suppose that for each $i \leq r$ the set of position of $w$ labelled with a satisfying $\varphi_i$ consists of at most $|\varphi_i|^2$ a-intervals. Then the number of endpoints of $a$-intervals comprising $J(w)$ is at most $4 + 2|\Sigma_1(\varphi_i)|^2$.

We first show how Lemma 3 follows from Lemma 7. We proceed by induction. The base step follows using the UAR, since for the predicate $b(x)$ the set $p(b, a)$ is either empty or a single $a$-interval. The cases for the boolean operations are routine.

In the induction step for existential quantification, we consider a formula $\psi(x) = \exists y \delta(x, y)$, where $\delta(x, y)$ is:

$$\beta(x \text{ DescOf } y, x = y, x \text{ AncOf } y, x \text{ InComp } y, \varphi_1, \ldots, \varphi_r, \rho_1, \ldots, \rho_s)$$

We can assume $\beta$ is normalized to be a disjunction of formulas $\beta_{\text{DescOf}}$, $\beta_{\text{AncOf}}$, $\beta_{\text{InComp}}$, $\beta_\text{=}$, where $\beta_{\text{DescOf}}(x, y)$ implies $y \text{ DescOf } x$, and similarly for the others. Thus in turn $\psi$ is the disjunction of $\psi_{\text{DescOf}}$, $\psi_{\text{AncOf}}$, $\psi_{\text{InComp}}$, $\psi_\text{=}$ where $\psi_R$ existentially quantifies over $\beta_R$.

For a boolean valuation $\sigma$ of the $\varphi_i$’s, and for a relation $R$ in $\text{DescOf}$, $\text{AncOf}$, $\text{InComp}$, $\text{=}$, we let $\delta(\sigma, R)(y)$ be the formula obtained from $\delta(x, y)$ by replacing all $\varphi_i(x)$ in $\delta$ by true or false according to $\sigma$, formula $R(x, y)$ by true, and all other binary formulas by false.

Fixing a root-to-leaf path $p = p_1 \ldots p_{\max(p)}$ in tree $t$ (that is, where $p_1$ is the root, $p_{\max(p)}$ a leaf), and $\sigma$ a boolean valuation of the $\varphi_i$’s let:

- $L_{\text{InComp}}(\sigma)$ represent the smallest $i$ such that
  $$\exists n \in t \cdot n \triangleleft \text{InComp} p_i \wedge t, n \models \delta(\sigma, \text{InComp})(y)$$

- $U_{\text{DescOf}}(\sigma)$ represent the largest $i$ such that
  $$\exists n \in t \cdot n \text{ DescOf } p_i \wedge t, n \models \delta(\sigma, \text{DescOf})(y)$$
- \( L_{\text{AncOf}}(\sigma) \) represent the smallest \( i \) such that

\[
\exists n \in t \cdot n \ \text{AncOf} \ p_i \land t, n \models \delta(\sigma, \text{AncOf})(y)
\]

Unwinding the definitions, we can check that a node \( p_j \) in the path \( p \) within \( t \) satisfies \( \psi \) exactly when, letting \( \sigma(j) \) be the boolean valuation of the \( \varphi_i \)'s such that \( t, p_j \models \varphi_i(x) \), we have either:
- \( j \leq U_{\text{DescOf}}(\sigma(j)) \) (thus \( p_j \) has a witness to \( \delta(\sigma(j), \text{DescOf}) \), and hence a witness to \( \psi \) which is a descendant).
- \( j \geq L_{\text{DescOf}}(\sigma(j)) \) (thus \( p_j \) has a witness to \( \psi \) that is incomparable to it).
- \( j \geq L_{\text{AncOf}}(\sigma(j)) \) (\( p_j \) has a witness to \( \psi \) which is an ancestor).
- \( t, p_i \models \psi_\leftarrow(x) \), where \( \psi_\leftarrow \) is defined above.

Restricting attention to \( \psi_{\text{DescOf}} \lor \psi_{\text{AncOf}} \lor \psi_{\text{InComp}} \), we can apply Lemma 7 above, letting \( L(\sigma) \) be the max of \( L_{\text{DescOf}}(\sigma) \) and \( L_{\text{AncOf}}(\sigma) \) and \( U(\sigma) \) be \( U_{\text{DescOf}}(\sigma) + 1 \).

We thus get that the number of boundary points of \( a \)-intervals comprising \( p(\psi_{\text{DescOf}} \lor \psi_{\text{AncOf}} \lor \psi_{\text{InComp}}, a) \) is at most \( 4 + 2(\Sigma_i|\varphi_i|)^2 \).

The boundary points of \( p(\psi_\leftarrow, a) \) are those of the \( p(\rho_i, a) \), and applying the induction hypothesis to these, we get a bound on the number of endpoints of intervals comprising \( p(\psi, a) \) as

\[
4 + 2(\Sigma_i|\varphi_i|)^2 + 2\Sigma_i|\rho_i|^2
\]

which is bounded by \( 2 \cdot |\psi|^2 \). Thus the number of intervals is bounded by \( |\psi|^2 \).

This completes the proof of Lemma 3.

We now proceed to the proof of Lemma 7.

We follow the approach of Lemma 2.1.10 of [Wei11] and focus on the modifications of the two main claims used in the proof of that lemma. For a formula \( \psi(x) \) and letter \( a \), let \( w(\psi, a) = \{ i \in w : w, i \models \psi(x) \land a(x) \} \).

For \( u \leq r \), let \( F_u \) be the set of left boundaries of \( a \)-intervals that comprise \( w(\varphi_u, a) \), and let \( G_u \) be the set of right interval boundaries, where (by convention) we take the decomposition into \( a \)-intervals of \( w(\varphi_u, a) \) to be such that the boundary points are labelled with \( a \), the right (upper) boundary is not part of \( w(\varphi_u, a) \) but the left boundary is in \( w(\varphi_u, a) \). Let \( F \) and \( G \) be the total set of left and right interval boundaries of \( S \), and let \( H = F \cup G \cup \{ 1, \|w\| + 1 \} \).

Consider each interval \( I \) defined by two consecutive elements of \( H \). The truth values of the \( \varphi_i \) are constant on such an interval, thus the truth value of \( \varphi \) on positions \( j \) in this interval is determined by where \( j \) is relative to \( L(\text{Val}(j)) \) and \( U(\text{Val}(j)) \). Let \( C \) be \( H \) unioned with all points of the form \( L(\text{Val}(j)) + 1 \) or \( U(\text{Val}(j)) \).

For a right (upper) interval boundary \( d \) in \( H \), we let \( q(d) \) be the point \( L(\text{Val}(j)) + 1 \) for \( j \) in the interval (all such points agree on \( \text{Val}(j) \)) to the left of \( d \), if such a point exists; \( q(d) \) is undefined otherwise. For a left (lower) interval boundary \( c \) in \( H \), we let \( p(c) \) be the point \( U(\text{Val}(j)) \) to the right of \( c \) within the interval, if it exists, and let \( p(c) \) be undefined otherwise. We let \( P(c) = p(c) \) exactly when \( p(c) \) is a right boundary point of \( J(w) \) – that is, an \( a \)-labelled position lying outside of the set, with the \( a \)-position immediately below it lying
in the set. Let $p(c)$ be undefined otherwise. Similarly let $Q(c) = q(c)$ when $q(c)$ is a left boundary point of $J(w)$.

Let $F_u$ be the union over all $F_v$ with $v \neq u$, and define $G_u$ analogously.

Claim. Given $c$ and $d$ consecutive interval boundaries from $F_u$, there is at most one $i \in F_u \cap [c,d)$ with $P(i) \neq \emptyset$.

Proof. Suppose there is $i \in F_u \cap [c,d)$ with $P(i) \neq \emptyset$ and consider another $j \in F_u \cap [c,d)$ with $j < i$. Since the interval $[c,d)$ contains no left interval boundaries besides the ones from $F_u$, and since $i$ and $j$ are both in $F_u$, and hence are both in $w(\varphi_u,a)$, we conclude that every $\varphi_k : k \leq r$ that holds in the interval starting from $i$ also holds at the interval starting from $j$. Thus $\text{Val}(j) = \text{Val}(i)$. If $p(j)$ is a right boundary point of $J(w)$, it must be that the positions immediately below it are in the set $J(w)$, and thus these positions must satisfy $x < U(\text{Val}(x))$. Once truth values for the $\varphi_k : k \leq r$ are fixed (and hence $\text{Val}(x)$ is fixed), the positions satisfying $x < U(\text{Val}(x))$ are closed downwards. Note that $i < p(i)$, by definition of $p(i)$, and therefore we must have that $i$ and $j$ both satisfy $x < U(\text{Val}(x))$. Combining with the fact that $i$ and $j$ agree on $\varphi_k : k \leq r$, we see that the interval above $j$ agrees on $J(w)$ with the interval above $i$, and thus $P(j)$ must be empty.

Let $C(i)$ be the set of boundary points contributed by $i$: namely $P(i)$ if it exists, $Q(i)$ if it exists, and also $i$ if it is a boundary point of $J(w)$.

Claim. Given $c$ and $d$ consecutive interval boundaries from $F_u$, and $i \in F_u \cap [c,d)$ with $i \notin G$, $Q(i) \neq \emptyset$. Then we have $i \notin C(i)$.

Proof. Fix $c, d, i$ as in the claim. Since $i \notin G$, $i$ is not a right interval boundary of any set $p(\varphi_j,a)$, and therefore the $\varphi_j$ that are true at the interval ending at $i$ are also true at the interval starting at $i$. Furthermore $Q(i) \neq \emptyset$ implies that $L(\text{Val}(x)) < x$ holds for $x$ above $Q(i)$, and thus will hold for all $a$-labelled positions sharing $\text{Val}(i)$ above $i$. Thus $i$ cannot be a boundary point for $J(w)$, and therefore $i \notin C(i)$.

The rest of the argument follows that in [Wei11] precisely.

The above two claims imply that for every $i \in F_u \cap [c,d) - G$ except possibly one element, $C(i)$ is either empty, contains the single element $Q(i)$, or contains only $i$. At the one exceptional element $C(i)$ could consist of at most two elements, $P(i)$ and either $Q(i)$ or $i$ (but not both, by the second claim).

Therefore, $\bigcup_{i \in F_u \cap [c,d) - G}$ has at most $|F_u \cap [c,d)| + 1$ elements. Unioning over all intervals $[c,d)$ we get

$$\Sigma_{i \in F_u - G}|C(i)| \leq \Sigma_{c \in F_u}(|F_u \cap [c,d)| + 1) = |F_u| + |F_u|$$

Using again the fact that each $C(i)$ contains at most two elements (see above), we also know $\Sigma_{i \in F_u - G}|C(i)| \leq 2 \cdot |F_u|$, and thus:

$$\Sigma_{i \in F_u - G}|C(i)| \leq |F_u| + \min\{|F_u|, |F_u|\}$$
Since for each $j$, the number of intervals, and hence the number of left endpoints of intervals, is assumed to be at most $|\phi_j|^2$, and using that the sum of squares is less than the square of a sum we get:

$$\sum_{i \in F_u - G} |C(i)| \leq |\phi_u|^2 + \min\{|\phi_u|^2, (\sum_{i \neq u} |\phi_i|)^2\} \leq |\phi_u|^2 + |\phi_u| \cdot \min\{|\phi_u|, \sum_{i \neq u} |\phi_i|\} \leq |\phi_u|^2 + |\phi_u| \cdot \sum_{i \neq u} |\phi_i| = |\phi_u| \cdot \sum_{i \neq u} |\phi_i|$$

By a symmetric argument we get

$$\sum_{i \in G_u - F} |C(i)| \leq |\phi_u| \cdot \sum_{i} |\phi_i|$$

Now the total number of boundary points for $J(w)$ is at most the endpoints of the path, the highest value of $U$ and the lowest value of $L$, plus the union over $i$ of $C(i)$. Thus we have that the total number is at most:

$$4 + \sum_a 2 \cdot |\phi_u| \cdot \sum_{i} |\phi_i| \leq 4 + 2 \cdot (\sum_i |\phi_i|)^2$$

This completes the proof of Lemma 7.

**Proof of Theorem 9**

Recall the statement:

*The satisfiability problem for FO$^2$[$V_{parOf}$] is NEXPTIME-hard, even with the unary alphabet restriction.*

*Proof.* Clearly, the UAR has no impact, since $n$ predicates on a single node can be simulated by considering the labels of the $n$ nearest ancestors.

We reduce from tiling a $2^n$ by $2^n$ grid with tiles $T_1 \ldots T_m$ in such a way to satisfy a given vertical constraint $V$ and horizontal constraint $H$. We let $\Sigma_n$ be an alphabet with symbols $ZeroX_1, OneX_1, \ldots, ZeroX_n, OneX_n, ZeroY_1, OneY_1, \ldots, ZeroY_n, OneY_n, T_1 \ldots T_m$. Consider trees in which: nodes at level $i \leq n$ are labelled with $ZeroX_i$ or $OneX_i$, each node of level $i \leq n - 1$ has both a $ZeroX_{i+1}$ and an $OneX_{i+1}$ child. Similarly nodes at level $n + 1 \leq i \leq 2n$ are labelled with $ZeroY_i$ or $OneY_i$. Each node of level $n$ has both $ZeroY_1$ and an $OneY_1$ child, each node of level $n + 1 \leq i \leq 2n - 1$ has both a $ZeroY_{i+1}$ and an $OneY_{i+1}$ child.

Finally, each node of level $2n$ has a single child labelled with one of the $T_i$. Such trees represent a tiling of the grid. It is easy to write an FO$^2$[$V_{parOf}$] formula describing such trees, and also requiring that the horizontal and vertical constraints are satisfied.

**Completion of the proof of Theorem 8**

Recall the statement:

*The satisfiability problem for FO$^2$[$V_{ancOf}$] over ranked schemas is in NEXPTIME, and is thus NEXPTIME-complete.*
We first prove the key lemma, Lemma 5. Recall that in this lemma, we replace node \( n \) by node \( n' \), where \( n \) and \( n' \) are not in the protected witness set \( W \) and share the same \( \varphi \)-type, the same set of ancestor \( \varphi \)-types, and the same set of selected descendant \( \varphi \)-types. The lemma then claims:

For all \( m \in T_1 \) the one-variable subformulas of \( \varphi \) satisfied by \( m \) in \( t \) are the same as those satisfied by \( f(m) \) in \( t' \). Moreover, for every node \( m' \) in \( T_2 \), the one-variable subformulas of \( \varphi \) satisfied by \( m' \) in \( t' \) are the same as those satisfied by \( f^{-1}(m') \) in \( t \).

We prove both parts of the lemma by simultaneous induction on the structure of the formula, where the case of atomic propositions and the case of boolean combinations are trivial. The only interesting case is for subformulas \( \exists y \beta(x, y) \).

We first note the following key property of the witness set \( W \): For nodes \( m \) of \( t \), if there is a \( w \) incomparable to \( m \) such that \( t, m, w \models \beta(x, y) \), then there is such a \( w \) in \( W \).

To prove this, fix \( m \) and \( w \) such that the hypothesis holds. Let \( w_\tau \) be the basic global witness for the \( \varphi \)-type of \( w \). If \( w_\tau \) is incomparable to \( m \), then \( w_\tau \) has the required property. If \( w_\tau \) is a descendant of \( m \), then we would have thrown in the necessary \( w \) into \( W \) as an incomparable global witness for \( m \). If \( w_\tau \) is an ancestor of \( m \) or equal to \( m \), we would have thrown in the necessary \( w \) into \( W \) as an incomparable global witness for \( w_\tau \).

We begin by comparing formulas \( \rho \) between a node \( m \) of the old tree (i.e. \( m \in T_1 \)) and the same node considered in the new tree. We first consider the case where \( \rho \) holds at \( m \) in \( t \), and show that \( \rho \) remains true at its image \( f(m) \) in \( t' \).

- If the witness of the truth of \( \psi \) was \( m \) or its ancestor, then these are also in \( T_1 \), and thus are preserved under the mapping, so by induction they (i.e. their image under \( f \)) can serve as a witness in \( t' \).
- Suppose there is a witness \( w \) that is neither \( m \), nor an ancestor of \( m \), nor a descendant of \( m \). By the key property of \( W \), there is a witness \( w' \) in the set \( W \) that is also incomparable to \( m \), and has the same \( \varphi \)-type as \( w \). This can be used as a witness.
- The last possibility is that some of the witnesses are descendants. If at least one of these is not in \( \text{SubTree}(t, n) \), then it is preserved and can be used as a witness. Otherwise, the witness must be in \( \text{SubTree}(t, n) \). If \( n \) itself was a witness, then since it was replaced by an \( n' \) such that \( \text{T}_p(\varphi)(n') = \text{T}_p(\varphi)(n) \) we can use the copy of \( n' \) as a witness, by induction. On the other hand, if there was a descendant of \( n \) which was a witness, then there would have been a witness \( w'' \) such that \( \text{T}_p(\varphi)(w'') \in \text{SelectedDescTypes}(n) \). Since \( \text{SelectedDescTypes}(n) = \text{SelectedDescTypes}(n') \), we would be able to find a witness with the appropriate \( \varphi \)-type in a copy of the subtree rooted at \( n' \).

We now consider the case where \( \rho \) holds at a node \( m' \) that is the image of a node \( m \) in \( \text{SubTree}(t, n') \) under the overwriting operation, and aim to show that \( \rho \) holds at \( m \). Note that once this is shown, the other direction of the if and only if for nodes in \( T_1 \) follows easily by induction. So fix such \( m' \) and \( m \). The only non-trivial case is for \( m' \) being a copy of \( n' \), with the witness being
its ancestor. Here we can use as a witness one of the ancestors of \( n \), because \( \text{AncTypes}(n) = \text{AncTypes}(n') \).

This completes the proof of Lemma 5. The argument for Theorem 8 for UAR trees proceeds by repeatedly updating while such nodes are available. The process terminates, as argued in the body of the paper.

The extension for ranked schemas follows along the same lines, but in order to collapse nodes \( n \) and \( n' \), we require in addition that the tree automaton \( A \) reaches the same state at \( n \) and \( n' \).

**Proof of Theorem 7**

Recall the statement:

There are \( \text{FO}^2[\text{V}_{\text{ancOf}}] \) formulas \( \varphi_n \) of size \( O(n) \) that are satisfiable over UAR binary trees, where the minimum depth of satisfying binary UAR trees grows as \( 2^n \).

*Proof.* We let \( \Sigma_n \) consist of \( \{b, s\} \cup \{a_i : i \leq n\} \).

We consider trees in which:
- the root is labelled \( b \)
- nodes labelled \( b \) are always comparable via descendant
- nodes labelled \( s \) are never comparable via descendant
- every ancestor of a \( b \)-labelled node is labelled \( b \)
- every ancestor of an \( s \)-labelled node is labelled \( b \)
- descendants of \( s \)-labelled nodes can be labelled with any of the \( a_i \) (but not with \( b \))

These conditions can easily be enforced by an \( \text{FO}^2[\text{V}_{\text{ancOf}}] \) formula.

In such trees the \( b \)-labelled nodes must go down a single branch, with \( s \)-labelled nodes splitting off on a separate branch. See Figure 2. We now let \( \psi_i : i \leq n \) be the formula that holds at an \( s \)-labelled node if it has a descendant \( a_i \). Note that any combination of the \( \psi_i \) are consistent, and the set of \( \psi_i \) that hold of an \( s \)-labelled node can thus be considered an \( n \)-bit address for the \( s \)-node. We can write a formula \( \varphi_n \) that asserts that 1. the constraint on the shape of the tree above holds 2. there is an \( s \)-node with address \( 0^n \) 3. for every \( s \)-labelled node with address \( a \) not equal to \( 1^n \), there is an \( s \)-labelled node whose bit address is the successor of \( a \). A binary tree satisfying \( \phi_n \) must have exponential depth. See Figure 2 for an example.

**Details for the proof of Theorem 10**

Recall the statement:

The satisfiability problem for \( \text{FO}^2[\text{V}_{\text{noAncOf}}] \), and the satisfiability problem with respect to a rank schema, are in \( \text{NEXPTIME} \), and hence are \( \text{NEXPTIME} \)-complete.

We give the details for satisfiability first. By Lemma 1 we know that a \( \text{FO}^2[\text{V}_{\text{noAncOf}}] \) formula \( \varphi \) which is satisfied over trees is satisfied by a tree \( t \) of depth at most exponential in \( \varphi \). We also can bound the outdegree of nodes by an exponential.
Fig. 2. An example model of exponential depth for FO$^2[V_{ancOf}]$ formula in ranked case

For each $\varphi$-type that is satisfied in $t$, choose a satisfier and include it along with all its ancestors in a set $W$: these are the basic witnesses. Then throw in all children of basic witnesses.

Thus the size of $W$ is at most exponential. Now we transform $t$ to another tree $t'$ such that $t' \models \varphi$ and $t'$ has only exponentially many different subtrees.

Recall that our update procedure looks for if there are nodes $n, n' \in t$ such that
1. $n, n' \notin W$
2. $\text{SubTree}(t, n) \not\sim \text{SubTree}(t, n')$ is not isomorphic to the subtree rooted at $n'$
3. $T_p(\varphi)(n) = T_p(\varphi)(n')$ and $T_p(\varphi)(\text{parent}(n)) = T_p(\varphi)(\text{parent}(n'))$
then let $t' = \text{Update}(t)$ be obtained by choosing such $n$ and $n'$ and applying the collapse operation that replaces the subtree of $n$ by that of $n'$.

Let $T_1$ be the nodes that were not in $\text{SubTree}(t, n)$, and for any node $m \in T_1$ let $f(m)$ denote the same node viewed in $t'$. Let $T_2$ denote the nodes in $t'$ that are images of a node in $\text{SubTree}(t, n')$ under the replacement. For each $m \in T_2$, let $f^{-1}(m)$ denote the node in $t$ from which it derives.

We claim the following:

**Lemma 8.** For all $m \in T_1$ the $\varphi$-type of $m$ in $t$ is the same as the $\varphi$-type of $f(m)$ in $t'$. Moreover, for every node $m' \in T_2$, the $\varphi$-type of $m'$ in $t'$ is the same as the $\varphi$-type of $f^{-1}(m)$ in $t$.

Applying the lemma above to the root of $t$, which is necessarily in $T_1$, it follows that the truth of the sentence $\varphi$ is preserved by this operation.

**Proof.** We prove both parts of the lemma by simultaneous induction on the structure of the formula, where the case of atomic propositions and the case of boolean combinations are trivial. The only interesting case is for subformulas $\psi = \exists y \beta(x, y)$.

We begin by considering formula $\psi$ at node $m \in T_1$. We first consider the case where $\varphi$ holds at $m$. 
– If the witness of the truth of \( \psi \) was \( m \) or its parent, then these are also in \( T_1 \), and thus are preserved under the mapping, so by induction they (i.e. their image under \( f \)) can served as a witness in \( t' \).
– Similarly, if the witness was a sibling of \( m \), then it can serve as a witness in \( t' \), since the collapse map does not impact the sibling relations.
– If all witnesses are neither a parent nor a child of \( m \), then take one such witness \( w \) and an element \( w' \) in \( W \) that realizes the same \( \varphi \)-type as \( w \). \( w' \) must be neither a parent or a child of \( m \) (since if it were a parent, \( m \) would have been a child witness, and hence protected). Thus \( w' \) can be used as a witness.
– The last possibility is that some of the witnesses are children. If at least one of these is not in \( \text{SubTree}(t, n) \), then it is preserved and can be used as a witness. Otherwise, \( n \) itself must be a witness. It was replaced by an \( n' \) such that \( Tp_\varphi(n) = Tp_\varphi(n') \) so the copy of \( n' \) can be used as a witness, by induction.

We now consider the case where \( \psi \) holds at a node \( m' \in T_2 \) that is the image of a node \( m \in T \), and aim to show \( \psi \) holds at \( m \). The only non-trivial case is for \( m' \) being the image of \( n' \), with the witness being its parent. Here we can use as a witness the parent of \( n \), because \( Tp_\varphi \) of the parent of \( n \) is the same as \( Tp_\varphi \) of the parent of \( n' \).

We now iterate the procedure \( t_{i+1} := \text{Update}(t_i) \), until no more updates are possible. Since \( t_{i+1} \prec t_i \), the process must terminate. The resulting tree will contain only exponentially many different subtrees. We can thus represent it as a DAG, with one node for each subtree.

Thus we have shown that any satisfiable formula has an exponential-size DAG that unfolds into a model of the formula. Given such a DAG, we can check whether an \( \text{FO}^2 \) formula holds in polynomial time in the size of the DAG. Thus we have a \textsc{NEXPTIME} algorithm for checking satisfiability.

The modification in the presence of a ranked schema is straightforward – again we show that there is an exponential-sized DAG. Given a bottom-up tree-automaton, the modification procedure \text{Update} only replaces \( n \) by \( n' \) if, in addition to the criteria above, their subtrees reach the same state of \( A \). Clearly, the state of \( A \) is also preserved by this replacement. This completes the proof of Theorem 10.