Bounds for the quantifier depth in finite-variable logics: Alternation hierarchy

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Given two structures $G$ and $H$ distinguishable in $\text{FO}^k$ (first-order logic with $k$ variables), let $A^k(G, H)$ denote the minimum alternation depth of a $\text{FO}^k$ formula distinguishing $G$ from $H$. Let $A^k(n)$ be the maximum value of $A^k(G, H)$ over $n$-element structures. We prove the strictness of the quantifier alternation hierarchy of $\text{FO}^2$ in a strong quantitative form, namely $A^2(n) > n/8 - 2$, which is tight up to a constant factor. For each $k \geq 2$, it holds that $A^k(n) > \log_{k+1} n - 2$ even over colored trees, which is also tight up to a constant factor if $k \geq 3$. For $k \geq 3$ the last lower bound holds also over uncolored trees, while the alternation hierarchy of $\text{FO}^2$ collapses even over all uncolored graphs.

We also show examples of colored graphs $G$ and $H$ on $n$ vertices that can be distinguished in $\text{FO}^2$ much more succinctly if the alternation number is increased just by one: while in $\Sigma_2$ it is possible to distinguish $G$ from $H$ with bounded quantifier depth, in $\Pi_2$ this requires quantifier depth $\Omega(n^2)$. The quadratic lower bound is best possible here because, if $G$ and $H$ can be distinguished in $\text{FO}^k$ with $i$ quantifier alternations, this can be done with quantifier depth $n^{2i-2} + 1$ and the same number of alternations.

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1. INTRODUCTION

Given structures $G$ and $H$ over vocabulary $\sigma$ and a first-order formula $\Phi$ over the same vocabulary, we say that $\Phi$ distinguishes $G$ from $H$ if $\Phi$ is true on $G$ but false on $H$. By alternation depth of $\Phi$ we mean the maximum length of a sequence of nested alternating quantifiers in $\Phi$. Obviously, this parameter is bounded from above by the quantifier depth of $\Phi$. We will examine the maximum alternation depth and quantifier depth needed to distinguish two structures for restrictions of first-order logic and particular classes of structures.

For a fragment $\mathcal{L}$ of first-order logic, by $A_{\mathcal{L}}(G, H)$ we denote the minimum alternation depth of a formula $\Phi \in \mathcal{L}$ distinguishing $G$ from $H$. Similarly, we let $D_{\mathcal{L}}(G, H)$...
denote the minimum quantifier depth of such \( \Phi \). Obviously, \( A_L(G, H) \leq D_L(G, H) \). We define the alternation function \( A_L(n) \) to be equal to the maximum value of \( A_L(G, H) \) taken over all pairs of \( n \)-element structures \( G \) and \( H \) distinguishable in \( L \).

Our interest in this function is motivated by the observation that if the quantifier alternation hierarchy of \( L \) collapses, then \( A_L(n) = O(1) \). More specifically, \( A_L(n) \leq a \) if the alternation hierarchy collapses to its \( a \)-th level \( \Sigma_a \cup \Pi_a \). Thus, showing that

\[
\lim_{n \to \infty} A_L(n) = \infty
\]

is a way of proving that the hierarchy is strict.

Note that Condition (1) is, in general, formally stronger than a hierarchy result. For example, while the alternation hierarchy of first-order logic \( \text{FO} \) is a way of proving that the hierarchy is strict. Note that any pair of structures \( S, T \) is distinguished from \( H \) by a formula \( \Phi \in L \) of the minimum alternation depth \( a \), then the set of structures \( L = \{ S : S \models \Phi \} \) is not definable in \( L \) with less than \( a \) quantifier alternations. Thus, the larger the value of \( A_L(n) \) is, the more levels of the alternation hierarchy can be separated by a certificate of size \( n \).

Results that we now know about the function \( A_L(n) \) are displayed in Figure 1. The upper bound \( A_{\text{FO}^k}(n) \leq n^{k-1} + 1 \) holds true even for the quantifier depth. This follows from the relationship of the distinguishability in \( \text{FO}^k \) to the count-free version of the \((k-1)\)-dimensional color refinement (Weisfeiler-Lehman) procedure discovered in [Immerman and Lander 1990; Cai et al. 1992]; see [Pikhurko and Verbitsky 2011]. For example, the \( \text{FO}^2 \)-equivalence type of an \( n \)-vertex graph can be defined based on [Immerman and Lander 1990, Theorem 1.8.1] and [Cai et al. 1992, Remark 5.5] with quantifier depth \( n + 1 \) because any color partition of an \( n \)-element set can be refined

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Fig. 1. Results about \( A_L(n) \). The upper bounds marked by * hold true even for the quantifier depth.
properly at most \( n - 1 \) times. Also the logarithmic upper bound for trees (Theorem 3.4) is actually proved for the quantifier depth.

Additionally, in Section 5 we show that the \( \Sigma_i \) fragment of \( \text{FO}^2 \) is not only strictly more expressive than the \( \Sigma_{i-1} \) fragment but also more succinct in the following sense: There are colored graphs \( G \) and \( H \) on \( n \) vertices such that they can be distinguished in \( \Sigma_{i-1} \cap \text{FO}^2 \) and, moreover, this is possible with bounded quantifier depth in \( \Sigma_i \cap \text{FO}^2 \) while in \( \Pi_i \cap \text{FO}^2 \) this requires quantifier depth \( \Omega(n^2) \). The quadratic lower bound is best possible here because, if \( G \) and \( H \) can be distinguished in \( \text{FO}^k \) with \( i \) quantifier alternations, this can be done with quantifier depth \( n^{2k-2} + 1 \) and the same number of alternations (Section 6).

A preliminary version of this paper appeared in [Berkholz et al. 2013].

2. PRELIMINARIES

2.1. Notation

We consider first-order formulas only in the negation normal form (i.e., any negation stands in front of a relation symbol and otherwise only monotone Boolean connectives are used). Given such a formula \( \Phi \), its set of sequences of nested quantifiers is denoted by \( \text{Nest}(\Phi) \) and defined by induction as follows:

1. If \( \Phi \) is quantifier-free, then \( \text{Nest}(\Phi) \) consists of the empty sequence;
2. \( \text{Nest}(\Phi \land \Psi) = \text{Nest}(\Phi) \cup \text{Nest}(\Psi) \), \( \text{Nest}(\Phi \lor \Psi) = \text{Nest}(\Phi) \cap \text{Nest}(\Psi) \);
3. \( \text{Nest}(\exists x \Phi) = \exists \text{Nest}(\Phi) \) and \( \text{Nest}(\forall x \Phi) = \forall \text{Nest}(\Phi) \), where \( \exists S \) (resp. \( \forall S \)) means the set of concatenations \( s \) (resp. \( \forall s \)) for all \( s \in S \).

The quantifier depth of a formula \( \Phi \) is the maximum length of a sequence in \( \text{Nest}(\Phi) \). The alternation depth of \( \Phi \) is the maximum number of alternating quantifier blocks in such a sequence.

For each \( i \geq 1 \), let \( \Sigma_i \) (resp. \( \Pi_i \)) denote the set of (not necessary prenex) formulas \( \Phi \) such that \( \Phi \) has alternation depth at most \( i \) and any sequence in \( \text{Nest}(\Phi) \) with \( i \) alternating quantifier blocks begins with \( \exists \) (resp. \( \forall \)). In particular, existential logic \( \Sigma_i \) consists of formulas without universal quantification. Note that \( \Sigma_i \cup \Pi_i \subset \Sigma_{i+1} \cap \Pi_{i+1} \). By the quantifier alternation hierarchy we mean the interlacing chains \( \Sigma_1 \subset \Sigma_2 \subset \ldots \) and \( \Pi_1 \subset \Pi_2 \subset \ldots \). We are interested in the corresponding fragments of a finite-variable logic.

Along with the notation \( A_{\leq}(G, H) \) and \( D_{\leq}(G, H) \) introduced in Section 1, we use shorthands \( D^k_{\leq}(G, H) = D^k_{\leq}(\text{FO}^k)(G, H) \) and \( A^k_{\leq}(G, H) = A^k_{\leq}(\text{FO}^k)(G, H) \). The subscript \( \text{FO} \) can be dropped; for example, \( D^k(G, H) = D^k_{\text{FO}}(G, H) \) and \( A^k(n) = A^k_{\text{FO}}(n) \). Sometimes we will write \( D^k_{\leq}(G, H) \) in place of \( D^k_{\Sigma_1}(G, H) \), and \( D^k_{\leq}(G, H) \) in place of \( D^k_{\Pi_1}(G, H) \).

We consider undirected graphs without loops. The first-order vocabulary for this class of structures consists of two binary relations, for adjacency and equality of vertices. For colored graphs, the vocabulary contains also unary relations for vertex colors. It is supposed that each vertex satisfies at most one color relation.

The vertex set of a graph \( G \) will be denoted by \( V(G) \), and the number of vertices in \( G \) will be denoted by \( v(G) \). A vertex is universal if it is adjacent to all other vertices.

2.2. The Ehrenfeucht-Fraïssé game

The \( k \)-pebble Ehrenfeucht-Fraïssé game on graphs \( G \) and \( H \) is played by two players, Spoiler and Duplicator, to whom we will refer as he and she, respectively. The players have equal sets of \( k \) pairwise different pebbles. A round consists of a move of Spoiler followed by a move of Duplicator. Spoiler takes a pebble and puts it on a vertex in \( G \) or in \( H \). Then Duplicator has to put her copy of this pebble on a vertex of the other
graph. Duplicator’s objective is to keep the following condition true after each round:
the pebbling should determine a partial isomorphism between $G$ and $H$. The variant
of the game where Spoiler starts playing in $G$ and is allowed to jump from one graph
to the other less than $i$ times during the game will be referred to as the $\Sigma_i$ game. In
the $\Pi_i$ game Spoiler starts in $H$.

For each positive integer $r$, the $r$-round Ehrenfeucht-Fraïssé game (as well as its $\Sigma_i$
and $\Pi_i$ variants) is a two-person game of perfect information with a finite number of
positions. Therefore, either Spoiler or Duplicator has a winning strategy
in this game, that is, a strategy winning against every strategy of the opponent.

**Lemma 2.1** (e.g., [Weis and Immerman 2009]). $D_{\Sigma_i}^k(G, H) \leq r$ if and only if
Spoiler has a winning strategy in the $r$-round $k$-pebble $\Sigma_i$ game on $G$ and $H$.

### 2.3. The lifting construction

Note that separation of the ground floor of the alternation hierarchy for $\text{FO}^2$ costs
nothing. We can take graphs $G$ and $H$ with three isolated vertices each, color one vertex
of $G$ in red, and color the other vertices of $G$ and all vertices of $H$ in blue. Obviously,
$D_{\Sigma_i}^2(G, H) = 1$ while $D_{\Pi_i}^2(G, H) = \infty$. It turns out that any separation example can be
lifted to higher floors in a rather general way. Similarly, given a sequence of examples
of $n$-vertex graphs $G$ and $H$ with $D_{\Sigma_i}^2(G, H) = \Omega(n^2)$ and $D_{\Pi_i}^2(G, H) = O(1)$, in Section 5
we will be able to lift it to any number of quantifier alternations.

The lifting gadget provided by Lemma 2.2 below is a reminiscence of the classical
construction designed by Chandra and Harel to prove the strictness of the first-order alternation hierarchy. The Chandra-Harel construction is applicable to other logics (see, e.g., [Ebbinghaus and Flum 1995, Section 8.6.3]), and can be used as a general scheme for obtaining hierarchy results. This approach was also used by Oleg Pikhurko (personal communication, 2007) to construct, for each $i$, a sequence of pairs of trees $G_n$ and $H_n$ such that $D_{\Sigma_i}^2(G_n, H_n) = O(1)$ while $D_{\Pi_i}^2(G_n, H_n) \to \infty$ as $n \to \infty$.

Given colored graphs $G_0$ and $H_0$, we recursively construct graphs $G_i$ and $H_i$ as shown
in Fig. 2. $H_1$ consists of three disjoint copies of $H_0$ and an extra universal vertex, that
will be referred to as the root vertex of $H_1$. The root vertex is colored in a new color
absent in $G_0$ and $H_0$, say, in gray. The graph $G_1$ is constructed similarly but, instead
of three $H_0$-branches, it has two $H_0$-branches and one $G_0$-branch. Suppose that $i \geq 1$
and the rooted graphs $G_i$ and $H_i$ are already constructed. The graph $H_{i+1}$ consists of
three disjoint copies of $G_i$ and the gray root vertex adjacent to the root of each $G_i$-part.
The graph $G_{i+1}$ is constructed similarly but, instead of three $G_i$-branches, it has two $G_i$-branches and one $H_i$-branch.

We will say that Spoiler plays continuously if, after each of his moves, the two pebbled vertices are adjacent.

**Lemma 2.2.** Assume that Spoiler has a continuous strategy allowing him to win the 2-pebble $\Sigma_1$ game on $G_0$ and $H_0$ in $r$ moves. Then, for each $i \geq 1$,

1. $D^2_{\Sigma_1}(G_i, H_i) < r + i$;
2. $D^2_{\Sigma_2}(G_i, H_i) \geq D^2_{\Pi_{i+1}}(G_i, H_i) \geq D^2_2(G_0, H_0)$;
3. $D^2_{\Pi_i}(G_i, H_i) = \infty$;
4. If, moreover, Spoiler has a continuous strategy allowing him to win the 2-pebble $\Sigma_2$ game on $G_0$ and $H_0$ in $s$ moves, then $D^2_{\Sigma_{i+1}}(G_i, H_i) < s + i$.

**Proof.** (1) In the base case of $i = 1$ we have to show that Spoiler is able to win the $\Sigma_1$ game on $G_1$ and $H_1$ in $r$ moves. He forces the $\Sigma_1$ game on $G_0$ and $H_0$ by playing continuously inside the $G_0$-part of $G_1$ and wins by assumption.

Now, we recursively describe a strategy for Spoiler in the $\Sigma_{i+1}$ game on $G_{i+1}$ and $H_{i+1}$, and inductively prove that it is winning. For each $i$, the strategy will be continuous, and the vertex pebbled in the first round will be adjacent to the root. Note that this is true in the base case.

In the first round Spoiler pebbles the root of the $H_i$-branch of $G_{i+1}$. Duplicator is forced to pebble the root of one of the $G_i$-branches of $H_{i+1}$. Indeed, if she pebbles a gray vertex at a different distance from the root of $H_{i+1}$, then Spoiler pebbles a shortest possible path upwards in $G_{i+1}$ or $H_{i+1}$, and wins once he reaches a non-gray vertex.

In the second round Spoiler jumps to this $G_i$-branch and, starting from this point, forces the $\Sigma_1$ game on $G_i$ and $H_i$ by playing recursively and, hence, continuously. The only possibility for Duplicator to avoid the recursive play and not to lose immediately is to pebble a gray vertex below. In this case Spoiler wins in altogether $i + 1$ moves by pebbling a path upwards in the graph where he stays, as already explained. If the game goes recursively, then by the induction assumption Spoiler needs less than $1 + r + i$ moves to win.

(2) In the base case of $i = 1$ we have to design a strategy for Duplicator in the $\Pi_2$ game on $G_1$ and $H_1$. First of all, Duplicator pebbles the gray vertex always when Spoiler does so. Furthermore, whenever Spoiler pebbles a vertex in an $H_0$-branch of $G_1$ or $H_1$, Duplicator pebbles the same vertex in an $H_0$-branch of the other graph. It is important that, if the pebbles are in two different $H_0$-branches of $G_1$ or $H_1$, Duplicator has a possibility to pebble different $H_0$-branches in the other graph. It remains to describe Duplicator’s strategy in the case that Spoiler moves in the $G_0$-branch of $G_1$. Note that once Spoiler does so, he cannot change the graph any more. In this case, Duplicator chooses a free $H_0$-branch in $H_1$ and follows her optimal strategy in the $\Sigma_1$ game on $G_0$ and $H_0$. Since the gray vertex is universal in both graphs and the $G_0$- and $H_0$-branches are isolated from each other, Spoiler wins only when he wins the $\Sigma_1$ game on $G_0$ and $H_0$, which is possible in $D^2_2(G_0, H_0)$ moves at the earliest.

In the $\Pi_{i+2}$ game on $G_{i+1}$ and $H_{i+1}$ Duplicator plays similarly. She always respects the root vertex, the $G_i$-branches, and takes care that the pebbled vertices are either in the same or in distinct $G_i$-branches in both graphs. Once Spoiler moves in the $H_i$-branch of $G_{i+1}$, Duplicator invokes her optimal strategy in the $\Sigma_{i+1}$ game on $H_i$ and $G_i$, what is the same as the $\Pi_{i+1}$ game on $G_i$ and $H_i$. There is no other way for Spoiler to win than to win this subgame. By the induction assumption, this takes at least $D^2_2(G_0, H_0)$ moves.

3. ALTERNATION FUNCTION FOR $\text{FO}^k$ OVER TREES

**Theorem 3.1.** $A^2(n) > \log_3 n - 2$ over colored trees.

**Proof.** Applying the lifting construction described in Section 2 to the pair of single-vertex graphs

$$G_0 = \bullet \quad \text{and} \quad H_0 = \circ,$$

we obtain the sequence of pairs of colored trees $G_i$ and $H_i$, with $v(G_i) = v(H_i)$ as shown in Fig. 3. For $i \geq 1$, we have

$$D^2_{\Sigma_i}(G_i, H_i) \leq i$$
Fig. 4. Proof of Theorem 3.2. The trees for 3-variable logic are still colored.

by part 1 of Lemma 2.2, and

\[ D_{\Pi_i}^2(G_i, H_i) = \infty \]

by part 3 of this lemma. It follows that \( G_i \) and \( H_i \) are distinguishable in \( \text{FO}^2 \) with alternation depth \( i \), but not with alternation depth \( i - 1 \). Thus, \( A^2(G_i, H_i) = i \). By the definition of the alternation function, \( A^2(n_i) \geq i \) for \( n_i = v(G_i) = v(H_i) \). Note that \( n_i = 3n_{i-1} + 1 \), where \( n_0 = 1 \). Therefore \( n_i = 3^i + \frac{3^i - 1}{2} \), which implies that \( A^2(n_i) > \log_3 n_i - 1 \).

Consider now an arbitrary \( n \) and suppose that \( n_i \leq n \leq n_i + 1 \). We can increase the number of vertices in \( G_i \) and \( H_i \) to \( n \) by attaching \( n - n_i \) new gray leaves at the root. This does not change the parameters \( D_{\Sigma_i}^2(G_i, H_i) \) and \( D_{\Pi_i}^2(G_i, H_i) \) because the new vertices help neither Duplicator in the \( \Sigma_i \) game nor Spoiler in the \( \Pi_i \) game. Spoiler can win the \( \Sigma_i \) game as before; pebbling a new grey vertex is a losing move for Duplicator because the distance to the leaves from this Duplicator’s pebble will be strictly larger than from the corresponding Spoiler’s pebble. If Spoiler decides to use a new vertex in the \( \Pi_i \) game, then Duplicator can mirror such a move on a new vertex in the other graph. Therefore, we get \( A^2(n) \geq A^2(n_i) > \log_3 n - 2 \).

Theorem 3.1 generalizes to any \( k \)-variable logic and, if \( k > 2 \), then no vertex coloring is needed any more.

**Theorem 3.2.** If \( k \geq 3 \), then \( A^k(n) > \log_{k+1} n - 2 \) over uncolored trees.

**Proof.** Notice that the lifting construction of Lemma 2.2 generalizes to \( k \geq 3 \) variables by adding \( k - 2 \) extra copies of \( H_0 \) in \( G_1 \) and \( H_1 \) and \( k - 2 \) extra copies of \( G_i \) in \( G_{i+1} \) and \( H_{i+1} \). Similarly to Theorem 3.1, this immediately gives us colored trees \( G_{i+1} \) and \( H_{i+1} \) such that \( D_{\Sigma_i}^2(G_i, H_i) \leq i \) and \( D_{\Pi_i}^2(G_i, H_i) = \infty \) for all \( i \geq 1 \); see Fig. 4.

In order to remove colors from \( G_i \) and \( H_i \), we construct these graphs recursively in the same way but now, instead of red and blue one-vertex graphs, we start with

\[
G_0 = \quad \text{and} \quad H_0 = \quad \text{see Fig. 5. Note that in the course of construction} \ G_0 \text{and} \ H_0 \text{will be handled as rooted trees (otherwise they are isomorphic).}
\]
We now claim that for the uncolored trees $G_i$ and $H_i$ it holds

1. $D_{1,i}^3(G_i, H_i) \leq i + 4$,
2. $D_{1,i}^k(G_i, H_i) = \infty$.

The latter claim is true exactly by the same reasons as in the colored case: since the number of Spoiler's jumps is bounded, Duplicator is always able to ensure playing on isomorphic branches. To prove the former claim, we will show that Spoiler can win similarly to the colored case playing with 3 pebbles.

Note that in the uncolored version of $G_i$ and $H_i$, all formerly gray vertices have degree $k + 1$, red vertices have degree 3, and blue vertices have degree 2. A typical ending of the game on the colored trees was that Spoiler pebbles a red vertex while Duplicator is forced to pebble a blue one. Now this corresponds to pebbling a vertex $u$ of degree 3 by Spoiler and a vertex $v$ of degree 2 by Duplicator. Having 4 pebbles, Spoiler would win by pebbling the three neighbors of $u$. Having only 3 pebbles, Spoiler first pebbles two neighbors $u_1$ and $u_2$ of $u$ (in fact, one neighbor is already pebbled immediately before $u$). Duplicator must respond with the two neighbors $v_1$ and $v_2$ of $v$. In the next round Spoiler moves the pebble from $u$ to its third neighbor $u_3$. Duplicator must remove the pebble from $v$ and place it on some vertex $v_3$ non-adjacent to both $v_1$ and $v_2$. Note that, while the distance between any two vertices of $u_1$, $u_2$, and $u_3$ equals 2, there is a pair of indices $s$ and $t$ such that $v_s$ and $v_t$ are at the distance more than 2. Spoiler now wins by moving the pebble from $u_q$ to $u_s$, where $\{q\} = \{1, 2, 3\} \setminus \{s,t\}$.

It remains to note that with 3 pebbles Spoiler is able to force climbing from the roots upwards in the trees and, hence, he can follow essentially the same winning strategy as in the colored case. Duplicator can deviate from this scenario only in the first round by pebbling a non-root vertex $v$ in $H_i$. In this case Spoiler pebbles, additionally to the root of $G_i$ pebbled in the first round, two its neighbors $u_1$ and $u_2$. If $i = 1$, both $u_1$ and $u_2$ have to correspond to formerly blue vertices. Duplicator must respond with two neighbors $v_1$ and $v_2$ of $v$. At least one of them, say $v_1$, is in the higher level than $v$. Then Spoiler uses his three pebbles to climb in $G_i$ from the root via $u_1$ to a leaf above a formerly blue vertex. Duplicator is forced to climb upwards in $H_i$ and loses because she reaches the highest possible level in $H_i$ sooner.

Thus, we have shown that $A^k(n_i) \geq i$ for $n_i = v(G_i)$. Since $n_i = (k + 1)n_{i-1} + 1$ and $n_0 = 3$, we have $n_i = 3(k + 1)^i + \frac{(k+1)^i-1}{k}$, which implies that $A^2(n_i) \geq \log_{k+1} n_i - 1$. Like in the proof of Theorem 3.1, this bound extends to all $n$ at the cost of decreasing it by 1. □

**Remark 3.3.** The proof of Theorem 3.2 implies that a limited number of quantifier alternations cannot be compensated by an increased number of variables: for every $k \geq 3$ and $i \geq 1$ there is a class of uncolored graphs definable in $\text{FO}^3$ but not in $\Sigma_i \cap \text{FO}^k$. If we allow vertex colors, there is such a class definable even in $\text{FO}^2$. 

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Fig. 5. Proof of Theorem 3.2. The uncolored versions of $G_1$ and $H_1$ for 3-variable logic.
Theorems 3.1 and 3.2 are optimal in the sense that they cannot be extended to FO^2 over uncolored trees. The reason is that the quantifier alternation hierarchy of FO^2 over uncolored graphs collapses to the second level; see Section 7.

We now show that the bound of Theorem 3.2 is tight up to a constant factor. The following theorem implies that, if k ≥ 3, then A^k(n) < (k + 3) log_2 n over colored trees. The proof easily extends to the class of all binary structures whose Gaifman graph is a tree.

**Theorem 3.4.** Let k ≥ 3. If D^k(T, T') < ∞ for colored trees T and T', then
\[ D^k(T, T') < (k + 3) \log_2 n \]
where n denotes the number of vertices in T.

**Proof.** Let T − v denote the result of removal of a vertex v from the tree T. The component of T − v containing a neighbor u of v will be considered a rooted tree with the root at u and called a branch of T at the vertex v. Let \( \tau(v) \) denote the maximum number of pairwise isomorphic branches at v. We define the branching index of T by \( \tau(T) = \max_v \tau(v) \). In order to prove the theorem, we will show that the bound (2) is true for any non-isomorphic colored trees with branching index at most k, and that \( D^k(T, T') = D^k(T \mod k, T' \mod k) \) for \( T \mod k \) and \( T' \mod k \) being “truncated” versions of T and T' whose branching index is bounded by k. We first handle the latter task.

The following fact easily follows from the trivial observation that k pebbles can be placed on at most k isomorphic branches.

**Claim 1.** Let T be a colored tree. Suppose that T has more than k isomorphic branches at a vertex v. Remove all but k of them from T and denote the resulting tree by \( \hat{T} \). Then \( D^k(T, G) = D^k(\hat{T}, G) \) for any colored graph G. \( \square \)

The truncated tree \( T \mod k \) is obtained from T by a series of truncations as in Claim 1. The truncation steps should be done from the top to the bottom in order to exclude appearance of new isomorphic branches in the course of the procedure. In order to define the “top” and “bottom” formally, recall that the eccentricity of a vertex v in a graph G is defined by \( e(v) = \max_u \text{dist}(v, u) \), where \( \text{dist}(v, u) \) denotes the distance between the two vertices. The diameter and the radius of G are defined by \( d(G) = \max_v e(v) \) and \( r(G) = \min_v e(v) \) respectively. A vertex v is central if \( e(v) = r(G) \). For trees it is well known (e.g., [Ore 1962, Chapter 4.2]) that if \( d(T) \) is even, then T has a unique central vertex c. If \( d(T) \) is odd, then T has exactly two central vertices \( c_1 \) and \( c_2 \), that are adjacent. Let us regard the central vertices as lying on the bottom level and the tree T as growing upwards. The height of a vertex is then its distance to the nearest central vertex. Starting from the highest level and going downwards, for each vertex v we cut off extra branches at v if their number exceeds k. Note that all “extra” branches of v grow upwards because v can have at most one branch whose vertices are not completely above the level of v. The cut-off operation can increase the number of isomorphic branches from vertices in lower levels but cannot do this for vertices in higher levels. Therefore, the resulting tree \( T \mod k \) has branching index at most k.

Applying Claim 1 repeatedly, we arrive at the equality \( D^k(T, T') = D^k(T \mod k, T' \mod k) \). Note that \( T \mod k \not\sim T' \mod k \) because it is assumed that \( D^k(T, T') < \infty \). Thus, we have reduced proving the bound (2) to the case that T and T' are non-isomorphic and both have branching index at most k. Therefore, below we make this assumption.
We have to show that Spoiler is able to win the k-pebble game on such T and T' in less than \((k + 3) \log_2 n\) moves. Below we will actively exploit the following fact, ensured by a standard halving strategy for Spoiler.

**Claim 2.** Suppose that in the 3-pebble Ehrenfeucht-Fraïssé game on graphs G and H some two vertices \(x, y \in V(G)\) at distance \(d\) are pebbled so that their counterparts \(x', y' \in V(H)\) are at a strictly larger distance. Then Spoiler can win in at most \(\lceil \log_2 d \rceil\) extra moves. □

We will use the following notation. Given two arbitrary vertices \(u\) and \(v\), let \(T_{u \setminus v}\) denote the tree obtained from \(T\) by rooting it at \(u\) and removing the branch (at the new root) containing \(v\). Note that if \(u\) and \(v\) are adjacent, then \(T_{u \setminus v}\) is a branch of \(T\) at \(v\). By \(N(w)\) we will denote the neighborhood of a vertex \(w\).

Every tree \(T\) has a single-vertex separator, that is, a vertex \(v\) such that no branch of \(T\) at \(v\) has more than \(n/2\) vertices; see, e.g., [Ore 1962, Chapter 4.2]. The idea of Spoiler’s strategy is to pebble such a vertex and to force further play on some non-isomorphic branches of \(T\) and \(T'\), where the same strategy can be applied recursively. This scenario was realized in [Pikhurko and Verbitsky 2011, Theorem 5.2] for first-order logic with counting quantifiers. Without counting, we have to use some additional tricks that are based on boundedness of the branching index.

Thus, in the first round Spoiler pebbles a separator \(v\) in \(T\) and Duplicator responds with a vertex \(v'\) somewhere in \(T'\). Suppose that \(v\) and \(v'\) have the same color. Since \(T \not\cong T'\), there is an isomorphism type \(B\) of a rooted tree that appears with different multiplicity among the branches of \(T\) at \(v\) and among the branches of \(T'\) at \(v'\).

**Claim 3.** Under the above conditions, Spoiler is able to force pebbling, additionally to the vertices \(v\) and \(v'\), a pair of their neighbors \(u \in N(v)\) and \(u' \in N(v')\) such that exactly one of the rooted trees \(T_{u \setminus v}\) and \(T'_{u' \setminus v'}\) has isomorphism type \(B\). This can be achieved with \(k\) pebbles in \(k + 1\) moves.

**Proof of Claim 3.** Denote the multiplicity of \(B\) at \(v\) by \(m\) and at \(v'\) by \(m'\). Suppose that \(m > m'\); the other case is symmetric. If \(m' \leq k - 2\), Spoiler pebbles \(m' + 1 < k\) roots of \(B\)-branches at \(v\); the vertices \(v\) and \(v'\) stay pebbled. Duplicator is forced to pebble \(m' + 1\) neighbors of \(v'\), and at least one of the corresponding branches has isomorphism type different from \(B\).

If \(m' > k - 2\), then \(m' = k - 1\) and \(m = k\). In this case Spoiler has to reuse the pebble on \(v\), as in the proof of Theorem 3.2. First he pebbles \(k - 1\) roots of \(B\)-branches at \(v\), keeping \(v\) pebbled. Duplicator is forced to respond with \(k - 1\) neighbors of \(v'\), but now those can be the roots of \(B\)-branches at \(v'\). In this case Spoiler moves the pebble from \(v\) to the remaining root \(u\) of a \(B\)-branch at \(v\). Denote Duplicator’s response by \(u'\). If \(u' \notin N(v')\), she loses in the next round. If \(u' \in N(v')\), then the isomorphism type of \(T'_{u' \setminus v'}\) differs from \(B\), and Spoiler moves one of the other pebbles back to \(v\). Duplicator is forced to move the other copy of this pebble to \(v'\). □

Using the strategy of Claim 3, Spoiler forces pebbling vertices \(u \in N(v)\) and \(u' \in N(v')\), with \(v\) and \(v'\) staying pebbled, so that the rooted trees \(T_{u \setminus v}\) and \(T'_{u' \setminus v'}\) are non-isomorphic. This phase of the game takes at most \(k + 2\) rounds.

The next goal of Spoiler is to force pebbling adjacent vertices \(v_1\) and \(u_1\) in \(T_{u \setminus v}\) and adjacent vertices \(v'_1\) and \(u'_1\) in \(T'_{u' \setminus v'}\) so that \(T_{u \setminus v} \not\cong T'_{u' \setminus v'}\) and

\[
v(T_{u \setminus v}) \leq v(T_{u \setminus v})/2 \text{ or } v(T'_{u' \setminus v'}) \leq v(T'_{u' \setminus v'})/2.\tag{3}
\]

Once this is done, the same will be repeated recursively (with the roles of \(T\) and \(T'\) swapped if only the second inequality in (3) is true).
Fig. 6. Proof of Theorem 3.4. Subcase 1-a: A branch of type \( B \) occurs in \( T_{w\setminus u} \) and, with different multiplicity (possibly 0), in \( T'_{w'\setminus w'} \). Subcase 1-b: Every branch of \( T_{w\setminus u} \) occurs with the same multiplicity in \( T'_{w'\setminus w'} \); a branch of type \( D \) occurs in \( T'_{w'\setminus w'} \), and does not in \( T_{w\setminus u} \).

To make the transition from \( T_{w\setminus u} \) to \( T_{w_1\setminus u_1} \), Spoiler first pebbles a separator \( w \) of \( T_{w\setminus u} \). Duplicator is forced to respond with a vertex \( w' \) in \( T'_{w'\setminus w'} \). Otherwise we would have \( \text{dist}(w, u) = \text{dist}(w, v) - 1 \) while \( \text{dist}(w', u') = \text{dist}(w', v') + 1 \). Therefore, some distances among the three pebbled vertices would be different in \( T \) and in \( T' \) and Spoiler could win in less than \( \log_2 \text{dist}(T_{w\setminus u}) + 1 \) moves by Claim 2.

Note that \( V(T_{w\setminus u}) \subset V(T_{w_1\setminus u_1}) \). We now consider two cases, depicted in Figures 6 and 7.

Case 1: \( T_{w\setminus u} \not\cong T'_{w'\setminus w'} \). In the trees \( T_{w\setminus u} \) and \( T'_{w'\setminus w'} \) we will consider branches at their roots \( w \) and \( w' \).

Subcase 1-a: \( T_{w\setminus u} \) contains a branch of isomorphism type \( B \) that has different multiplicity in \( T'_{w'\setminus w'} \). Similarly to Claim 3, Spoiler can use \( k \) pebbles and \( k + 1 \) moves to force pebbling, additionally to the vertices \( w \) and \( w' \), their neighbors \( x \in N(w) \) and \( x' \in N(w') \) such that \( T_{x\setminus w} \not\cong T'_{x'\setminus w'} \) and

\[
T_{x\setminus w} \in B \text{ or } T'_{x'\setminus w'} \in B
\]  
(4)

(the pebbles occupying \( v, v' \) and \( u, u' \) can be released). The branches \( T_{x\setminus w} \) and \( T'_{x'\setminus w'} \) will now serve as \( T_{u_1\setminus v_1} \) and \( T'_{u'_1\setminus v'_1} \). Condition (3) follows from (4) because \( w \) is a separator of \( T_{w'\setminus u} \).
Subcase 1-b: $T_{w\setminus u}$ does not contain any branch as in Subcase 1-a. In this subcase there is a vertex $x' \in N(w')$ such that $T'_{x'\setminus w'}$ is a branch of $T_{w\setminus u'}$ and the isomorphism type of $T'_{x'\setminus w'}$ does not appear in $T_{w\setminus u}$. Notice a difference to Subcase 1-a: There is no guarantee now that $v(T'_{x'\setminus w'})$ is bounded by $v(T_{w\setminus v})/2$. Spoiler moves the pebble from $v'$ to $x'$. Suppose that Duplicator responds with $x \in N(w)$. Since $T'_{x'\setminus w'}$ is a branch of $T_{w\setminus u'}$, the vertex $x'$ does not lie on the path between $u'$ and $w'$. If $x$ lies on the path between $u$ and $w$, then equality of distances among the pebbled vertices cannot be preserved, and Spoiler wins by Claim 2. For a vertex $y$ on the path between $u$ and $w$, let $T_y\setminus u,w$ denote the tree obtained from $T$ by rooting it at $y$ and removing the branches (at the new root) containing $u$ and $w$. The rooted tree $T_y\setminus u,w$ is defined similarly. Note that $T_w\setminus v,w$ and each $T_y\setminus u,w$ are parts of a branch of $T_w\setminus v$ at the vertex $w$ and, therefore, have at most $v(T_w\setminus v)/2$ vertices. Given $y$ between $u$ and $w$, by $y'$ we will denote the vertex lying between $u'$ and $w'$ at the same distance to these vertices as $y$ to $u$ and $w$. We suppose that $y$ and $y'$ have the same color for else Spoiler wins by Claim 2. Since $T_{u\setminus v} \not= T_{w\setminus u'}$, we must have

$$T_y\setminus u,w \not= T'_y\setminus u',w'$$

(5)

for some $y$, or

$$T_w\setminus v,w \not= T'_w\setminus v',w'.$$

(6)

Assume that Condition (5) is true for some $y$ and fix this vertex.

Subcase 2-a: $T_y\setminus u,w$ contains a branch of isomorphism type $B$ that has different multiplicity in $T_y\setminus u,w$. Spoiler moves the pebble from $v$ to $y$. Duplicator is forced to move the pebble from $v'$ to $y'$. The pebbles occupying $u, u'$ and $w, w'$ can now be released. Spoiler proceeds similarly to Subcase 1-a and forces pebbling vertices $z \in N(y)$ and $z' \in N(y')$ such that $T_{z\setminus y} \not= T'_{z'\setminus y'}$ and one of these trees has isomorphism type $B$ and, hence, is as small as desired.

Subcase 2-b: $T_y\setminus u,w$ does not contain any branch as in Subcase 2-a. In this subcase there is a vertex $z' \in N(y')$ such that $T_{z'\setminus y'}$ is a branch of $T'_{y\setminus u',w'}$ whose isomorphism type does not appear in $T_{y\setminus u,w}$. Similarly to Subcase 1-b, Spoiler aims to pebble $y'$ and $z'$ while forcing Duplicator to respond with $y$ and $z \in N(y)$ such that $T_{z\setminus y}$ is a part of $T_{y\setminus u,w}$. This will ensure that $T_{z\setminus y} \not= T'_{z'\setminus y'}$ and that $T_{z\setminus y}$ is small enough. Now Spoiler’s task is more complicated because he has to prevent Duplicator from pebbling $z$ on the path between $u$ and $w$. Since this requires keeping the pebbles on $u, u'$ and $w, w'$, Spoiler cannot pebble both $y'$ and $z'$ if there are only $k = 3$ pebbles. In this case he first pebbles the vertex $z'$ by the pebble released from $v$. Let $z$ be the Duplicator’s response. If $z$ is in $N(y)$ and does not lie between $u$ and $w$, Spoiler succeeds by moving the pebble from $u'$ to $y'$. Duplicator is forced to move the pebble from $u$ to $y$ because $w'$ remains pebbled and, therefore, the position of $y$ is determined by the distances to $z$ and $w$. If $z$ is not in $N(y)$ or lies between $u$ and $w$, then Spoiler wins because dist($z,u$) $\not= dist(z',u')$ or dist($z,w$) $\not= dist(z',w')$.

An analysis of the case (6) is quite similar. The role of the triple $(u,y,w)$ is now played by the triple $(v,u,w)$. 

Fig. 7. Proof of Theorem 3.4. Case 2: $T_{w \backslash v} \cong T'_{w' \backslash v'}$. Subcase 2-a: A branch of type $B$ occurs in $T_{y \backslash u, w}$, and, with different multiplicity (possibly 0), in $T'_{y' \backslash u', w'}$. Subcase 2-b: Every branch of $T_{y \backslash u, w}$ occurs with the same multiplicity in $T'_{y' \backslash u', w'}$; a branch of type $C$ occurs in $T'_{y' \backslash u', w'}$ and does not in $T_{y \backslash u, w}$.

Note that the transition from $T_{u \backslash v}$ to $T_{u_1 \backslash v_1}$ takes at most $k + 3$ rounds. Also, 2 rounds suffice to win the game once the current subtree $T_{u \backslash v}$ has at most 2 vertices. The number of transitions from the initial branch, having at most $n/2$ vertices, to one with at most 2 vertices is bounded by $\log_2 n - 1$ because $v(T_{u \backslash v})$ becomes twice smaller each time. It follows that Spoiler wins the game on $T$ and $T'$ in less than $k + 2 + (\log_2 n - 1)(k + 3) + 2 \leq (k + 3) \log_2 n + 1$ moves. The additive term of 1 can be dropped because if pebbling the initial branch takes no less than $k + 2$ moves, then the size of this branch will actually not exceed $n/k$. Note, finally, that if Duplicator deviates from the above scenario and forces Spoiler to use the strategy of Claim 2, she cannot resist longer. If this happens after pebbling the $r$-th version of $T_{u \backslash v}$, having still more than 2 (but no more than $n/2$) vertices, Claim 2 is applied in the situation when the distance between the two Spoiler’s pebbles is less than $n/2$. Then the total duration of the game is less than $(k + 2) + (r - 1)(k + 3) + 3 + [\log_2 (n/2')] < r(k + 2) + 3 + \log_2 n$ rounds, which is less than $\log_2 n(k + 3)$ because $r \leq \log_2 n - 1$.

4. ALTERNATION FUNCTION FOR $\text{FO}^2$ OVER COLORED GRAPHS

Theorem 3.1 gives us a logarithmic lower bound on the alternation function $A^2(n)$, which holds even for trees. Over all colored graphs, we now prove a linear lower bound. Along with the general upper bound $A^2(n) \leq n + 1$, it shows that $A^2(n)$ has linear growth.

**Theorem 4.1.** $A^2(n) > n/8 - 2$.

**Proof.** For each integer $m \geq 2$, we will construct colored graphs $G$ and $H$, both with $n = 8m - 4$ vertices, that can be distinguished in $\text{FO}^2$ with $m - 2$, but no less
than that, alternations. The graph \( G = 2G_m \) is the union of two disjoint copies of the same graph \( G_m \) and, similarly, \( H = 2H_m \) where \( G_m \) and \( H_m \) are defined as follows. Each of \( G_m \) and \( H_m \) is obtained by merging two building blocks \( A_m \) and \( B_m \) shown in Fig. 8. The colored graph \( A_m \) is a “ladder” with \( m \) horizontal rungs, each having 2 vertices. The vertices on the bottom rung are colored in green, the vertices on the top rung are colored one in red and the other in blue, the remaining \( 2m - 4 \) vertices are white (uncolored). The graph \( B_m \) is obtained from \( A_m \) by recoloring red in apricot and blue in cyan. \( A_m \) and \( B_m \) are glued together at the green vertices. There are two ways to do this, and the resulting graphs \( G_m \) and \( H_m \) are non-isomorphic. Let \( \alpha^+ \) (resp. \( \alpha^- \)) denote the partial isomorphism from \( G_m \) to \( H_m \) identifying the \( A_m \)-parts (resp. the \( B_m \)-parts) of these graphs.

We will design a strategy allowing Spoiler to win the \( (m - 2) \)-alternation (i.e., \( \Sigma_{m-1} \) or \( \Pi_{m-1} \)) 2-pebble Ehrenfeucht-Fraïssé game on \( G \) and \( H \), and a strategy allowing Duplicator to win the \( (m - 3) \)-alternation game. Before playing on \( G \) and \( H \), we analyze the 2-pebble game on \( G_m \) and \( H_m \). Spoiler can win this game as follows. In the first round he pebbles the left green vertex in \( G_m \); see Fig. 8. Not to lose immediately, Duplicator responds either with the left or with the right green vertex in \( H_m \). The corresponding partial isomorphism can be extended to \( \alpha^+ \) in the former case and to \( \alpha^- \) in the latter case (but not to both \( \alpha^+ \) and \( \alpha^- \)). These two cases are similar, and we consider the latter of them, where there is no extension to \( \alpha^+ \) and hence Spoiler has a chance to win playing in the \( A_m \)-parts of \( G_m \) and \( H_m \).

In the second round Spoiler pebbles the upright neighbor of the left green vertex in \( G_m \). His goal in subsequent rounds is to force pebbling, one by one, edges along the upright paths to the red vertex in \( G_m \) and to the blue vertex in \( H_m \). If Duplicator makes a step down, Spoiler wins by reaching the top rung sooner than Duplicator. If Duplicator moves upward all the time, starting from the third round of the game she has a possibility to slant. Spoiler prevents this by changing the graph. Note that in one of the graphs there is only one way upstairs, and Spoiler always leaves this graph for Duplicator. In this way Spoiler wins by making \( m \) moves and alternating between the graphs \( m - 2 \) times.

The strategy we just described is inoptimal with respect to the alternation number. In fact, Spoiler can win the game on \( G_m \) and \( H_m \), with no alternation at all by pebbling...
in the first round the right green vertex in $G_m$. If Duplicator responds with the left green vertex in $H_m$, Spoiler puts the second pebble on the non-adjacent vertex in the next upper rung. Duplicator is forced to play in a different rung of $H_m$ because otherwise she would violate the non-adjacency relation. If in the first round Duplicator responds with the right green vertex, Spoiler plays similarly, but in the lower rung of $G_m$. In any case, the second pebble is closer to the red or to the apricot vertex in $G_m$ than in $H_m$, which makes Spoiler’s win easy.

Nevertheless, the former, $(m - 2)$-alternation strategy has an advantage: Spoiler ensures that the two pebbled vertices are always adjacent. By this reason, the same strategy can be used by Spoiler to win also the game on $G = 2G_m$ and $H = 2H_m$. Once Duplicator steps aside to another copy of $G_m$ or $H_m$, she immediately loses.

The partial isomorphism $\alpha^+_{m}$ from $G_m$ to $H_m$ determines two partial isomorphisms $\alpha^+_0$ and $\alpha^+_1$ from $G = 2G_m$ to $H = 2H_m$ identifying the two $A_m$-parts of $G$ with the two $A_m$-parts of $H$. Similarly, $\alpha^-$ gives rise to two partial isomorphisms $\alpha^-_0$ and $\alpha^-_1$.

We now show that the number of alternations $m - 2$ is optimal for the game on $G$ and $H$. Fix an integer $a$ such that Spoiler has a winning strategy in the $a$-alternation 2-pebble game on $G$ and $H$. For this game, let us fix an arbitrary winning strategy for Spoiler and a strategy for Duplicator satisfying the following conditions.

— Duplicator always respects vertex rungs (this is clearly possible because every rung in $G$ and $H$ has four vertices and there are only two pebbles).

— Additionally, Duplicator respects adjacency (this is possible and complies with the preceding rule because there are edges only between adjoining rungs and every vertex sends at least one edge to each adjoining rung).

— Duplicator respects also non-adjacency. Moreover, whenever Spoiler violates adjacency of the vertices pebbled in one graph, Duplicator responds so that the vertices pebbled in the other graph are not only non-adjacent but even lie in different $G_m$- or $H_m$-components.

— If Spoiler pebbles a vertex above the green rung and the three preceding rules still do not determine Duplicator’s response uniquely, then she responds according to $\alpha^+_0$ or $\alpha^-_1$; in a similar situation below the green rung, she plays according to $\alpha^-_0$ or $\alpha^+_1$.

Note that these rules uniquely determine Duplicator’s moves on non-green vertices provided one pebble is already on the board. In particular, the choice of $\alpha^+_0$ or $\alpha^-_1$ in the last rule depends on the component where this pebble is placed.

Let $u_i \in V(G)$ and $v_i \in V(H)$ denote the vertices pebbled in the $i$-th round of the game. We now highlight a crucial property of Duplicator’s strategy. Suppose that $u_i$, $v_i$ and $u_{i+1}$, $v_{i+1}$ are in the $A_m$-parts of $G$ and $H$ and that $u_{i+1}$ and $v_{i+1}$ are non-green. Then the following conditions are met.

— If $u_i$ and $u_{i+1}$ (as well as $v_i$ and $v_{i+1}$) are non-adjacent, then $\alpha^+_s(u_{i+1}) = v_{i+1}$ for $s = 0$ or $s = 1$.

— If $u_i$ and $u_{i+1}$ (as well as $v_i$ and $v_{i+1}$) are adjacent and $\alpha^+_s(u_i) = v_i$ for $s = 0$ or $s = 1$, then $\alpha^-_s(u_{i+1}) = v_{i+1}$ for the same $s$.

A similar property holds if the pebbles are in the $B_m$ parts.

Suppose that Spoiler wins in the $r$-th round. Note that Duplicator’s strategy allows Spoiler to win only when $u_r$ and $v_r$ are in the top or in the bottom rungs and have different colors (in the absence of these colors, the described strategy would be winning for Duplicator). Since the two cases are similar, assume that Spoiler wins on the top.

Let $p$ be the smallest index such that all vertices in the sequence $u_p$, $v_p$, ... , $u_r$, $v_r$ are above the green level. By assumption, $\alpha^+_r(u_r) \neq v_r$ for both $s = 0, 1$. The aforemen-
tioned property of Duplicator’s strategy implies that, furthermore,
\[ \alpha_0^+(u_i) \neq v_i \text{ and } \alpha_1^+(u_i) \neq v_i \text{ for all } i \geq p. \] (7)

Therefore, \( u_{i+1} \) and \( u_i \), as well as \( v_{i+1} \) and \( v_i \), are adjacent for all \( i \geq p \) (for else Duplicator plays so that \( \alpha_1^+(u_{i+1}) = v_{i+1} \) for \( s = 0 \) or \( s = 1 \)). By the same reason, \( p > 1 \), and \( u_{p-1} \) and \( v_{p} \) are also adjacent. It follows that \( u_{p-1} \) and \( v_{p-1} \) are green and \( \alpha_s^+(u_{p-1}) \neq v_{p-1} \) for both \( s = 0, 1 \).

Another consequence of (7) is that both vertex sequences \( u_{p-1}, u_{p}, \ldots, u_r \) and \( v_{p-1}, v_p, \ldots, v_r \) lie on upright paths. This follows from the fact that either from \( u_i \) or from \( v_i \) there is only one edge emanating upstairs (also downstairs), and it is upright.

It remains to notice that after each transition to the adjoining rung (i.e., from \( u_i, v_i \) to \( u_{i+1}, v_{i+1} \) for \( i \geq p - 1 \)) Spoiler has to jump to the other graph because otherwise Duplicator will choose the neighbor that ensures \( \alpha_s^+(u_{i+2}) = v_{i+2} \) for some value of \( s = 0, 1 \) (determined by the condition that \( \alpha_s^+ \) is a map from the component of \( G \) containing \( u_{p-1} \) to the component of \( H \) containing \( v_{p-1} \)). This observation readily implies that the number of alternations \( a \) cannot be smaller than \( m - 2 \).

We have shown that \( A^2(n) \geq m - i \) if \( n = 8m - 4 \). Adding up to seven isolated vertices to both \( G \) and \( H \), we get the same bound also for \( n = 8m - 3, \ldots, 8m + 3 \). Therefore, \( A^2(n) \geq (n - 11)/8 \) for all \( n \).

\[ \square \]

5. LOWER BOUNDS FOR \( D^2_k(G, H) \) AND SUCCINCTNESS RESULTS

5.1. Existential two-variable logic

In the next section we will see that, if structures \( G \) and \( H \) have \( n \) elements each and \( G \) is distinguishable from \( H \) in existential two-variable logic, then \( D^2_k(G, H) \leq n^2 + 1 \).

Here we show that this bound is tight up to a constant factor. For the existential-positive fragment of \( FO^2 \), a quadratic lower bound can be obtained from the benchmark instances for the arc consistency problem going back to [Dechter and Pearl 1985; Samal and Henderson 1987]; see [Berkholz and Verbitsky 2013], where also an alternative approach is suggested. Here, we elaborate on the construction presented in [Berkholz and Verbitsky 2013]. To implement this idea for existential two-variable logic, we need to undertake a more delicate analysis as the existential-positive fragment is more restricted and simpler.

**Theorem 5.1.** For an arbitrarily large \( n \) there exist \( n \)-vertex colored graphs \( G \) and \( H \) such that \( G \) is distinguishable from \( H \) in existential two-variable logic and

\[ D^2_k(G, H) > \frac{1}{16} n^2. \]

**Proof.** Our construction will depend on an integer parameter \( m \geq 2 \). We construct a pair of colored graphs \( G_m \) and \( H_m \), such that \( G_m \) is distinguishable from \( H_m \) in existential two-variable logic, both \( v(G_m) = O(m) \) and \( v(H_m) = O(m) \), and \( D^2_k(G_m, H_m) = \Omega(m^2) \). Though \( v(G_m) < v(H_m) \), later we will be able to increase the number of vertices in \( G_m \) to \( v(H_m) \).

The graphs have vertices of 4 colors, namely apricot, blue, cyan, and dandelion. \( G_m \) contains a cycle of length \( 3(2m - 1) \) where apricot, blue, and cyan alternate as shown in Fig. 9. \( H_m \) contains a similar cycle of length \( 3 \cdot 2m \). Successive apricot, blue, and cyan vertices will be denoted by \( a_i, b_i, \) and \( c_i \) in \( G_m \), where \( 0 \leq i < 2m - 1 \), and by \( a'_i, b'_i, \) and \( c'_i \) in \( H_m \), where \( 0 \leq i \leq 2m - 1 \). Furthermore, the vertex \( a_0 \) is adjacent to a dandelion vertex \( d_0 \), and every \( a'_i \) except for \( i = m \) is adjacent to a dandelion vertex \( d'_i \). This completes the description of the graphs.

By Lemma 2.1, we have to show that Spoiler is able to win the 2-pebble \( \Sigma_1 \) game on \( G_m \) and \( H_m \) and that Duplicator is able to prevent losing the game for \( \Omega(m^2) \) rounds.
Note that, once the pair \((a_0, a'_m)\) is pebbled, Spoiler wins in the next move by pebbling \(a_0\). He is able to force pebbling \((a_0, a'_m)\) as follows. In the first round he pebbles \(a_0\). Suppose that Duplicator responds with \(a'_s\), where \(0 \leq s < m\). In a series of subsequent moves, Spoiler goes around the whole circle in \(G_m\), visiting \(c_{2m-2}, b_{2m-2}, a_{2m-2}, c_{2m-3}, \ldots\) and using the two pebbles alternately (if \(m < s < 2m\), he does the same but in the other direction). As Spoiler comes back to \(a_0\), Duplicator is forced to arrive at \(a'_{s+1}\). The next Spoiler’s tour around the circle brings Duplicator to \(a'_{s+2}\), and so forth. Thus, the most successful move for Duplicator in the first round is \(a'_0\). Then Spoiler needs to play \(1 + m \cdot 3(2m - 1) + 1 = 6m^2 - 3m + 2\) rounds in order to win.

Our next task is to design a strategy for Duplicator allowing her to survive \(\Omega(m^2)\) rounds, no matter how Spoiler plays. We will show that Duplicator is able to force Spoiler to pass around the cycle in \(G_m\) many times. A crucial observation is that \((a_0, a'_m)\) is the only pair whose pebbling allows Spoiler to win in one extra move.

Let us regard the additive group \(\mathbb{Z}_{2m}\) as a cycle graph with \(i\) and \(j\) adjacent iff \(i - j = \pm 1\). Denote the distance between vertices in this graph by \(\Delta\). The same letter will denote the following partial function \(\Delta : V(G_m) \times V(H_m) \rightarrow \mathbb{Z}\). For two vertices of the same color, say, for \(a_i, a'_i\), we set \(\Delta(a_i, a'_i) = \Delta(i, j)\). Note that \(\Delta(a_0, a'_m) = m\), which is the largest possible value. Duplicator’s strategy will be to keep the value of the \(\Delta\)-function on the pebbled pair as small as possible.

Specifically, in the first round Duplicator responds to Spoiler’s move \(x\) with pebbling a vertex \(x'\) such that \(\Delta(x, x') = 0\) (that is, if \(x = a_i, b_i, c_i, d_i\), then \(x' = a'_i, b'_i, c'_i, d'_i\) respectively). Suppose that a pair \((y, y')\) is pebbled in the preceding round and Duplicator is still alive. If Spoiler pebbles \(x\) in the current round, Duplicator chooses her response \(x'\) by the following criteria. Below, \(\sim\) denotes the adjacency relation.

- \(x'\) should have the same color as \(x\) and, moreover, \(x' \sim y'\) iff \(x \sim y\) (this is always possible unless \((y, y') = (a_0, a'_m)\) and \(x = d_0\));
- if there is still more than one choice, \(x'\) should minimize the value \(\Delta(x, x')\).

We do not consider the cases when \(x = y\) or when \(x\) is pebbled by the pebble removed from \(y\) because, in our analysis, we can assume that Spoiler uses an optimal strategy, allowing him to win the 2-pebble \(\Sigma_1\) game on \(G_m\) and \(H_m\) from the initial position \((y, y')\) in the smallest possible number of rounds (if he does not play optimally, Duplicator survives even longer).

**Claim 4.** If \(x \neq y\) and \(x \neq y\), then \(\Delta(x, x') \leq 1\).
Proof of Claim 4. Assume first that $x \neq d_0$ and $y \neq d_0$. W.l.o.g., suppose that $y$ and $y'$ are apricot and, specifically, $y' = a_j'$ (the blue and the cyan cases are symmetric to the apricot case). Not to lose immediately, Duplicator cannot pebble $x'$ in \{c_{j-1}, a_j', b_j'\}, where $j-1$ is supposed to be an element of $Z_{2m}$. This can obstruct attaining $\Delta(x, x') = 0$ (if $x \in \{c_{j-1}, a_j, b_j\}$), but then there is a choice of $x'$ with $\Delta(x, x') = 1$.

Assume now that $x = d_0$. Then $x' = d_0'$ if $y' \neq a_0'$ and $x' = d_1'$ otherwise. In both cases $\Delta(x, x') \leq 1$.

Finally, let $y = d_0$ and $y' = d_0'$. Then the value $x' = a_j'$ is forbidden and, if this prevents $\Delta(x, x') = 0$, then we have $\Delta(x, x') = 1$. $\square$

Consider now the dynamical behaviour of $\Delta(x, x')$, assuming that Duplicator uses the above strategy and Spoiler follows an optimal winning strategy. We have $\Delta(x, x') = 0$ at the beginning of the game and $\Delta(x, x') = m$ at the end (that is, in the round immediately before Spoiler wins). Consider the last round of the game where $\Delta(x, x') \leq 1$. By Claim 4, starting from the next round Spoiler always moves along an edge in $G_m$. Note that, from now on, visiting $d_0$ earlier than in the very last round would be inoptimal. Therefore, Spoiler walks along the circle. Another consequence of optimality is that he always moves in the same direction.

W.l.o.g., we can suppose that Spoiler moves in the ascending order of indices. Note that $\Delta(x, x')$ increases by 1 only under the transition from $x = a_{2m-2}$ to $x = a_0$ (at this point, the index of $x$ makes a jump in $Z_{2m}$, while the index of $x'$ moves along $Z_{2m}$ always continuously). In order to increase $\Delta(x, x')$ from 1 to $m$, the edge $a_{2m-2}a_0$ must be passed $m-1$ times. It follows that, before Spoiler wins, the game lasts at least $2 + (m - 2) \cdot 3(2m - 1) = 6m^2 - 15m + 8$ rounds.

Note that $v(G_m) = 6m - 2$ and $v(H_m) = 8m - 1$. In order to make the number of vertices in both graphs $n = 8m - 1$, let $m$ be a multiple of 3 and add two new connected components to $G_m$, namely the cycle of length $2m$ with alternating colors apricot, blue, and cyan and one isolated vertex of any color. Spoiler can still win by playing in the old component. Since playing in the new components does not help him, the game on the modified $G_m$ and the same $H_m$ lasts at least $6m^2 - 15m + 8 = \frac{4}{3} \cdot n^2 - O(n)$ rounds.

Remark 5.2. In order to facilitate the exposition, the construction of graphs $G_m$ and $H_m$ uses 4 colors. In fact, the same idea can be realized with 2 colors. This is optimal because for uncolored graphs one can show, using our analysis of this case in Section 7, that if $G$ is distinguishable from $H$ in existential two-variable logic, then $D^2_{\Sigma_i}(G, H) \leq 2v(H)$.

5.2. Lifting it higher
Since $D^2_{\Sigma_i}(G, H) = D^2_{\Sigma_i}(H, G)$, the results of this section hold true as well for $\Pi_i \cap \text{FO}^2$.

Theorem 5.3. Let $i \geq 1$. For an arbitrarily large $n$ there exist $n$-vertex colored graphs $G$ and $H$ such that $G$ is distinguishable from $H$ in $\Sigma_i \cap \text{FO}^2$ and $D^2_{\Sigma_i}(G; H) > \frac{1}{1129} \cdot n^2 - \frac{1}{1152} \cdot n$.

Proof. For infinitely many values of an integer parameter $n_0$, Theorem 5.1 provides us with colored graphs $G_0$ and $H_0$ on $n_0$ vertices each such that Spoiler has a continuous winning strategy in the 2-pebble $\Sigma_1$ game on $G_0$ and $H_0$, and $D^2_{\Sigma_1}(G_0, H_0) > \frac{1}{1129} \cdot n_0^2$. Let $G_i$ and $H_i$ be now the graphs obtained from $G_0$ and $H_0$ by the lifting construction described in Section 2. Note that $v(G_i) = 3v(G_{i-1}) + 1$, where $G_0 = G$. It follows that $n = v(G_i) = 3^in_0 + \frac{3^i - 1}{2}$. The graph $G_i$ is distinguishable from $H_i$ in $\Sigma_i \cap \text{FO}^2$ by part 1 of Lemma 2.2. By part 2 of this lemma, we have $D^2_{\Sigma_i}(G_i, H_i) > \frac{1}{1152} \cdot n_0^2$, which implies the bound stated in terms of $n$. $\square$
An analog of Theorem 5.3 can be shown for uncolored directed graphs by appropriately modifying Theorem 5.1 and Lemma 2.2. However, Theorem 5.3 cannot be extended to uncolored undirected graphs because in this case our results in Section 7 imply that, if $G$ is distinguishable from $H$ in $FO^2$, then $D_{Σ_2}^k(G, H) ≤ max\{v(G), v(H)\}$.

Using a similar sequence of graphs, we can also show that $Σ_i ∩ FO^2$ is more succinct than $Σ_{i-1} ∩ FO^2$. Given $i$, let us construct $G_i$ and $H_i$ starting from $G_0$ and $H_0$ as in the proof of Theorem 5.3, with the only difference that all dandelion vertices in $H_0$ are now adjacent. The modification of $H_0$ allows Spoiler to win the $Σ_2$ game on $G_0$ and $H_0$ using a simple continuous strategy: He just pebbles two dandelion vertices in $H_0$. This makes part 4 of Lemma 2.2 applicable, which along with part 2 gives us the following result.

**Theorem 5.4.** Let $i ≥ 2$. For an arbitrarily large $n$ there exist $n$-vertex colored graphs $G$ and $H$ such that $D_{Σ_i}^k(G, H) = O(1)$ while $D_{Σ_{i-1}}^k(G, H) < ∞$ and $D_{Π_i}^k(G, H) = Ω(n^2)$.

6. AN UPPER BOUND FOR $D_{Σ_i}^k(G, H)$

Since $D_{Σ_i}^k(G, H) = D_{Π_i}^k(H, G)$, the following result holds true as well for $Π_i ∩ FO^k$. Moreover, it admits a direct generalization to arbitrary relational structures.

**Theorem 6.1.** Let $G$ and $H$ be colored graphs. If $G$ is distinguishable from $H$ in $Σ_i ∩ FO^k$, then $D_{Σ_i}^k(G, H) ≤ (v(G)v(H))^{k-1} + 1$.

**Proof.** By Lemma 2.1, we have to prove that, if Spoiler has a winning strategy in the $r$-round $k$-pebble $Σ_i$ game on $G$ and $H$ for some $r$, then he has a winning strategy in the game with $(v(G)v(H))^{k-1} + 1$ rounds.

The proof is based on a general game-theoretic argument. Consider a two-person game, where the players follow some fixed strategies and one of them wins. Then the length of the game cannot exceed the total number of all possible positions because once a position occurs twice, the play falls into an endless loop. This argument assumes that the players’ strategies are positional, that is, that a strategy of a player maps a current position (rather than the sequence of all previous positions) to one of the moves available to the player.

Implementing this scenario for the $Σ_i$ game, we have to overcome two complications. First, we have to “reduce” the space $V(G)^k × V(H)^k$ of all possible positions in the game, which has size $(v(G)v(H))^k$. Second, we have take care of the fact that, if $i > 1$, then Spoiler’s play can hardly be absolutely memoryless in the sense that he apparently has to remember the number of jumps left to him or, at least, the graph in which he moved in the preceding round.

We begin with some notation. Let $\bar{u}$ and $\bar{v}$ be tuples of vertices in $G$ and $H$, respectively, having the same length of no more than $k$. Given $Ξ ∈ \{Σ, Π\}$ and $a ≥ 1$, let $R(Ξ, a, \bar{u}, \bar{v})$ be the minimum $r$ such that Spoiler has a winning strategy in the $Ξ_a$ game on $G$ and $H$ starting from the initial position $(\bar{u}, \bar{v})$. Given a $k$-tuple $\bar{w}$ and $j ≤ k$, let $σ_j\bar{w}$ denote the $(k - 1)$-tuple obtained from $\bar{w}$ by removal of the $j$-th coordinate. Note that, if $\bar{u} ∈ V(G)^k$ and $\bar{v} ∈ V(H)^k$, then

$$R(Ξ, a, \bar{u}, \bar{v}) = \min_{1 ≤ j ≤ k} R(Ξ, a, σ_j\bar{u}, σ_j\bar{v}) .$$

In order to estimate the length of the $k$-pebble $Σ_a$ game on $G$ and $H$, we fix a strategy for Duplicator arbitrarily and consider the strategy for Spoiler as described below. For $i ≥ 1$, we will say that $Ξ_s = (Ξ_s, a_s, \bar{u}_s, \bar{v}_s)$ is the position after the $s$-th round if

- $Ξ_s = Σ$ if in the $s$-th round Spoiler moved in $G$ and $Ξ_s = Π$ if he moved in $H$;
— during the first $s$ rounds Spoiler jumped from one graph to another $i - a_s$ times;
— after the $s$-th round the pebbles $p_1, \ldots, p_k$ are placed on the vertices $\bar{u} \in V(G)^k$ and $\bar{v} \in V(H)^k$ (we suppose that in the first round Spoiler puts all $k$ pebbles on one vertex).

Furthermore, we will say that $\tilde{C}_s = (\Xi_s, a_s, \bar{u}_s, \bar{v}_s)$ is the position before the $(s + 1)$-th move if in the $(s + 1)$-th round Spoiler moves the pebble $p_j$ and $\bar{u}_s = \sigma_j \bar{u}_s$ and $\bar{v}_s = \sigma_j \bar{v}_s$.

Let us describe Spoiler’s strategy. He makes the first move according to an arbitrarily prescribed strategy that is winning for him in the $D^k_{\Sigma_1}(G, H)$-round $k$-pebble $\Sigma_1$ game on $G$ and $H$. If this move is in $G$, let $\Xi_1 = \Sigma$ and $a_1 = 1$; otherwise $\Xi_1 = H$ and $a_1 = i - 1$.

After Duplicator responds, the position $C_1$ is specified. Note that $R(C_1) < D^k_{\Sigma_1}(G, H)$.

Suppose that the $s$-th round has been played and after this we have the position $\tilde{C}_s = (\Xi_s, a_s, \bar{u}_s, \bar{v}_s)$. In the next round Spoiler plays with the pebble $p_j$ for the smallest value of $j$ such that

$$R(\tilde{C}_s) = R(\tilde{C}_s).$$

Such index $j$ exists by (8). Spoiler makes his move according to a prescribed strategy that is winning for him in the $R(\tilde{C}_s)$-round $k$-pebble $(\Xi_s) a_s$ game on $G$ and $H$ with the initial position $(\bar{u}_s, \bar{v}_s)$. If he moves in the same graph as in the $s$-th round, then $\Xi_{s+1} = \Xi_s$ and $a_{s+1} = a_s$; otherwise $\Xi_{s+1}$ gets flipped and $a_{s+1} = a_s - 1$.

Note that $a_{s+1} < a_s$ and, if $\Xi_{s+1} \neq \Xi_s$, then $a_{s+1} < a_s$. Since Spoiler in each round uses a strategy optimal for the rest of the game,

$$R(\tilde{C}_{s+1}) < R(\tilde{C}_s).$$

It follows, in particular, that the described strategy is winning for Spoiler in the $\Sigma_i$ game on $G$ and $H$.

We now estimate the length of the game from above. Suppose that after the $t$-th round Duplicator is still alive. Due to (9) and (10),

$$R(\tilde{C}_1) > R(\tilde{C}_2) > \ldots > R(\tilde{C}_t).$$

It follows that the elements of the sequence $\tilde{C}_1, \tilde{C}_2, \ldots, \tilde{C}_t$ are pairwise distinct. We conclude from here that the elements of the sequence $(\bar{u}_1, \bar{v}_1), (\bar{u}_2, \bar{v}_2), \ldots, (\bar{u}_t, \bar{v}_t)$ are pairwise distinct too. Indeed, let $s' > s$. If $a_{s'} = a_s$, then $\Xi_s = \Xi_{s'}$. Since $\tilde{C}_s \neq \tilde{C}_{s'}$, we have $(\bar{u}_s, \bar{v}_s) \neq (\bar{u}_{s'}, \bar{v}_{s'})$. If $a_{s'} < a_s$, the same inequality follows from the fact that $R(\Xi, a, \bar{u}, \bar{v}) \leq R(\Xi', a', \bar{u}, \bar{v})$ whenever $a' < a$.

Since $(\bar{u}_s, \bar{v}_s)$ ranges over $V(G)^{k-1} \times V(H)^{k-1}$, we conclude that $t \leq (v(G)v(H))^{k-1}$ and, therefore, Spoiler wins in the round $(v(G)v(H))^{k-1} + 1$ at the latest. □

7. THE COLLAPSE OF THE ALTERNATION HIERARCHY OF $\text{FO}^2$ OVER UNCOLORED GRAPHS

We here show that the quantifier alternation hierarchy of $\text{FO}^2$ over uncolored graphs collapses to the second level. To prove this result, we first introduce combinatorial characteristics of an uncolored graph that capture its $\text{FO}^2$-equivalence class.

7.1. Ranking and types of uncolored graphs

The complement of a graph $G$ is the graph on the same vertex set $V(G)$ with any two vertices adjacent if and only if they are not adjacent in $G$. We call a graph normal if it has neither isolated nor universal vertices. Note that a graph is normal iff its complement is normal. For every graph $G$ with at least 2 vertices we inductively define its rank $\text{rk} G$:

— Graphs of rank 1 are exactly the empty, the complete, and the normal graphs.
Graphs of rank 2 are exactly the graphs obtained by adding universal vertices to empty graphs, or isolated vertices to complete graphs, or either universal or isolated vertices to normal graphs.

— If $i \geq 2$, disconnected graphs of rank $i + 1$ are obtained from connected graphs of rank $i$ by adding a number of isolated vertices.

— For every $i \geq 2$, connected graphs of rank $i$ are exactly complements of disconnected graphs of rank $i$.

A simple inductive argument on the number of vertices shows that all graphs with at least two vertices get ranked. Indeed, if a graph $G$ is normal, complete, or empty, it receives rank 1. This includes the case that $G$ has two vertices. If $G$ does not belong to any of these three classes, it has either isolated or universal vertices. Since graphs with universal vertices are connected and are the complements of graphs with isolated vertices, it suffices to consider the case that $G$ has isolated vertices. Remove all of them from $G$ and denote the result by $G'$. Note that $G'$ has less vertices than $G$ but still more than one vertex. By the induction assumption, $G'$ is ranked. If $\text{rk} G' = 1$, that is, $G'$ is complete or normal, then $\text{rk} G = 2$ by definition. Suppose that $\text{rk} G' > 1$. Since $G'$ is not normal and has no isolated vertex, this graph must have a universal vertex and, hence, is connected. Therefore, $\text{rk} G = \text{rk} G' + 1$ by definition.

We now introduce a ranking of vertices in a graph $G$. If $\text{rk} G = 1$, then all vertices of $G$ get rank 1. Suppose that $\text{rk} G > 1$. If $G$ is disconnected, it has at least one isolated vertex; if $G$ is connected, there is at least one universal vertex. Denote the set of such vertices by $\partial G$. Every vertex in $\partial G$ is assigned rank 1. If $u \notin \partial G$, then it is assigned rank one greater than the rank of $u$ in the graph $G - \partial G$. The rank of a vertex $u$ in $G$ will be denoted by $\text{rk} u$. It ranges from the lowest value 1 to the highest value $\text{rk} G$. Note that a vertex $u$ with $\text{rk} u < \text{rk} G$ has the same adjacency to all other vertices of equal or higher rank.

Given an integer $m \geq 1$ and a graph $G$ with $\text{rk} G > m$, we define the $m$-tail type of $G$ to be the sequence $(t_0, t_1, \ldots, t_m)$ where $t_0 \in \{\text{conn, disc}\}$ depending on whether $G$ is connected or disconnected and, for $i \geq 1$, $t_i \in \{\text{thin, thick}\}$ depending on whether there is a single vertex of rank $i$, or there are at least two such vertices.

Furthermore, we define the kernel of a graph $G$ to be its subgraph induced on the vertices of rank $\text{rk} G$. Note that the kernel of any $G$ is a graph of rank 1. We define the head type of $G$ to be $\text{empty, complete, or normal}$ depending on the kernel. We say that graphs $G$ and $H$ are of the same type if $\text{rk} G = \text{rk} H$, $G$ and $H$ have the same head type, and if $\text{rk} G > 1$, then they also have the same $m$-tail type for $m = \text{rk} G - 1$. The single-vertex graph has its own type.

**Lemma 7.1.**

1. If $G$ and $H$ are of the same type, then $D^2(G, H) = \infty$.
2. If $G$ and $H$ have the same $m$-tail type, then $D^2(G, H) \geq m$.

**Proof.** (1) Let $\text{rk} G = \text{rk} H = m + 1$. Let $V(G) = U_1 \cup \ldots \cup U_{m+1}$ and $V(H) = V_1 \cup \ldots \cup V_{m+1}$ be the partitions of the vertex sets of $G$ and $H$ according to the ranking of vertices. We will describe a winning strategy for Duplicator in the two-pebble game on $G$ and $H$. We will call a pair of pebbled vertices $(u, v) \in V(G) \times V(H)$ straight if $u \in U_i$ and $v \in V_j$ for the same $i$. Note that both the kernels $U_{m+1}$ and $V_{m+1}$ contain at least 2 vertices and, since $G$ and $H$ are of the same type, $|U_i| = 1$ iff $|V_i| = 1$. This allows Duplicator to play so that the vertices pebbled in each round form a straight pair and the equality relation is never violated. If the head type of $G$ and $H$ is empty or complete, this strategy is winning because the adjacency of vertices $u \in U_i$ and $u' \in U_j$ depends only on the indices $i$ and $j$ and is the same as the adjacency of any vertices $v \in V_i$ and $v' \in V_j$. It remains to notice that Duplicator can resist also when the game is played...
inside the normal kernels $U_{m+1}$ and $V_{m+1}$. In this case she never loses because, for every vertex in a normal graph, she can find another adjacent or non-adjacent vertex, as she desires.

(2) We have to show that Duplicator can survive for at least $m - 1$ rounds. Note that both $rk G \geq m + 1$ and $rk H \geq m + 1$. Similarly to part 1, consider partitions $V(G) = U_1 \cup \ldots U_{m+1}$ and $V(H) = V_1 \cup \ldots V_{m+1}$, where $U_{m+1}$ and $V_{m+1}$ now consist of the vertices whose rank is higher than $m$. In the first round Duplicator plays so that the pebbled vertices form a straight pair. However, starting from the second round it can be for her no longer possible to keep the pebbled pairs straight. Call a pair of pebbled vertices $(u, v) \in V(G) \times V(H)$ skew if $u \in U_i$ and $v \in V_j$ for different $i$ and $j$. Assume that Spoiler uses his two pebbles alternatingly (playing with the same pebble in two successive rounds gives him no advantage). Let $(u_r, v_r)$ denote the pair of vertices pebbled the $r$-th round. If $(u_r, v_r)$ is skew, let $S_r$ denote the minimum $s$ such that $u_r \in U_s$ or $v_r \in V_s$. If $(u_r, v_r)$ is straight, we set $S_r = m + 1$. Our goal is to show that, if $S_r = m + 1$, then Duplicator has a non-losing move in the next round such that $S_{r+1} \geq m - 1$ and that, as long as $1 < S_r \leq m$, she has a non-losing move such that $S_{r+1} \geq S_r - 1$. This readily implies that Duplicator does not lose the first $m - 1$ rounds.

To avoid multiple treatment of symmetric cases, we use the following notation. Let $\{G_1, G_2\} = \{G, H\}$. Let $y_1 \in G_1$ and $y_2 \in G_2$ denote the vertices being pebbled in the round $r + 1$, and let $x_1 \in G_1$ and $x_2 \in G_2$ be the vertices pebbled in the round $r$ (in the previous notation, $\{x_1, x_2\} = \{u_r, v_r\}$ and $\{y_1, y_2\} = \{u_{r+1}, v_{r+1}\}$).

Suppose first that $\{x_1, x_2\}$ is a straight pair contained in the slice $U_i \cup V_i$. If $i \leq m$, it makes no problem for Duplicator to move so that the pair $\{y_1, y_2\}$ is also straight. This holds true also if $i = m + 1$ and Spoiler pebbles $y_a \in U_j \cup V_j$ with $j \leq m$. Thus, in these cases $S_{r+1} = S_r = m + 1$. However, if $i = j = m + 1$, moving straight can always make Duplicator lose the game. In this case she survives by pebbing a vertex $y_{3-a}$ of rank $m$ or $m - 1$, depending on the adjacency relation between $x_a$ and $y_a$. In this case $S_{r+1} \geq m - 1$.

Let us accentuate the property of the vertex ranking that is beneficial to Duplicator in the last case. Recall that, if a vertex $u$ is not in the graph kernel, it has the same adjacency to all other vertices of equal or higher rank. If $u$ is adjacent to all such vertices, we say that $u$ is of universal type; otherwise we say that it is of isolated type. Duplicator uses the fact that the type of a vertex gets flipped when its rank increases by one.

Suppose now that $\{x_1, x_2\}$ is a skew pair. Let $x_1 \in U_i \cup V_i$ and $x_2 \in U_j \cup V_j$ and, w.l.o.g., assume that $i > j$. Note that $j = S_r$ and recall that $S_r > 1$. Consider three cases depending on Spoiler's move $y_a$. In the case most favorable for Duplicator, $rk y_a < j$. Then Duplicator responds with a vertex $y_{3-a}$ of the same rank, resetting $S_{r+1}$ back to the initial value $m + 1$. If Spoiler pebbles a vertex $y_2$ of $rk y_2 \geq j$, then Duplicator responds with a vertex $y_1$ of $rk y_1 = j$, keeping $S_{r+1} \geq j = S_r$ (unchanged or reset to $m + 1$). Finally, consider the case when Spoiler pebbles a vertex $y_1$ of $rk y_1 \geq j$. Assume that $x_2$ is of universal type (the other case is symmetric). If $y_1$ and $x_1$ are adjacent, then Duplicator responds with a vertex $y_2$ of $rk y_2 = i$, keeping $S_{r+1} \geq S_r$. If $y_1$ and $x_1$ are not adjacent, then Duplicator responds with $y_2$ of $rk y_2 = j - 1$, which is of isolated type. This is the only case when $S_{r+1} = S_r - 1$ decreases. 

\textbf{Lemma 7.2.}

\begin{enumerate}
  \item For each $m$-tail type, the class of graphs of this type is definable by a first-order formula with two variables and one quantifier alternation.
  \item For each $G$, the class of graphs of the same type as $G$ is definable by a first-order formula with two variables and one quantifier alternation.
\end{enumerate}
PROOF. (1) Consider an \( m \)-tail type \((t_0, t_1, \ldots, t_m)\). Assume that \( t_0 = \text{conn} \) (the case of \( t_0 = \text{disc} \) is similar). Let \( \sim \) denote the adjacency relation. We inductively define a sequence of formulas \( \Phi_s(x) \) with occurrences of two variables \( x \) and \( y \) and with one free variable:

\[
\begin{align*}
\Phi_1(x) & \overset{\text{def}}{=} \forall y (y \sim x \lor y = x), \\
\Phi_{2k}(x) & \overset{\text{def}}{=} \forall y (\Phi_{2k-1}(y) \lor y \not\sim x), \\
\Phi_{2k+1}(x) & \overset{\text{def}}{=} \forall y (\Phi_{2k}(y) \lor y \sim x \lor y = x).
\end{align*}
\]

Here \( \Phi_{2k-1}(y) \) is obtained from \( \Phi_{2k}(x) \) by swapping \( x \) and \( y \). A simple inductive argument shows that, if \( G \) is a connected graph and \( \text{rk} \, G \) is greater than an odd (resp. even) integer \( s \), then \( G, v \models \Phi_s(x) \) exactly when the vertex \( v \) is of universal (resp. isolated) type and \( \text{rk} \, v \leq s \).

Furthermore, we define a sequence of closed formulas \( \Psi_s \), with alternation number 1:

\[
\begin{align*}
\Psi_1 & \overset{\text{def}}{=} \exists x \Phi_1(x) \land \exists x \sim \Phi_{1}(x), \\
\Psi_2 & \overset{\text{def}}{=} \exists x \Phi_1(x) \land \exists x \Phi_{2}(x) \land \exists x (\neg \Phi_1(x) \land \neg \Phi_{2}(x)), \\
\Psi_s & \overset{\text{def}}{=} \exists x \Phi_1(x) \land \exists x \Phi_{2}(x) \land \bigwedge_{i=3}^{s} \exists x (\Phi_1(x) \land \neg \Phi_{i-2}(x)) \land \exists x (\neg \Phi_{s-1}(x) \land \neg \Phi_s(x)),
\end{align*}
\]

where \( s \geq 3 \). Note that a graph \( G \) satisfies \( \Psi_s \) if and only if \( G \) is connected and \( \text{rk} \, G > s \).

We are now able to define the class of graphs of \( m \)-tail type \((t_0, t_1, \ldots, t_m)\) by the conjunction

\[
\Psi_m \land \bigwedge_{i=1}^{m} T_i,
\]

where

\[
T_i \overset{\text{def}}{=} \exists x \exists y (x \not\sim y \land \Phi_i(x) \land \neg \Phi_{i-2}(x) \land \Phi_{i}(y) \land \neg \Phi_{i-2}(y))
\]

if \( t_i \) is \textit{thick} and

\[
T_i \overset{\text{def}}{=} \forall x \forall y (\neg \Phi_i(x) \lor \neg \Phi_{i}(y) \lor \Phi_{i-2}(x) \lor \Phi_{i-2}(y) \lor x = y)
\]

if \( t_i \) is \textit{thin} (if \( i \leq 2 \), the subformulas with non-positive indices should be ignored).

(2) The single-vertex graph is defined by a formula \( \forall x \forall y (x = y) \). The three classes of graphs of rank 1 are defined by the following three formulas:

\[
\begin{align*}
\exists x \exists y (x \not\sim y) \land \forall x \forall y (x \not\sim y), \\
\exists y \forall y (x \not\sim y) \land \forall x \forall y (x = y \lor x \sim y), \\
\forall x \exists y (x \sim y) \land \forall x \exists y (x \not\sim y \land x \not\sim y).
\end{align*}
\]

Suppose that \( \text{rk} \, G = m+1 \) and \( m \geq 1 \). Let \((t_0, t_1, \ldots, t_m)\) be the \( m \)-tail type of \( G \). Assume that \( G \) is connected, that is, \( t_0 = \text{conn} \) (the disconnected case is similar). We use the formulas \( \Phi_s(x) \), \( \Psi_s \), and \( T_i \) constructed in the first part. If the head type of \( G \) is \textit{complete} or \textit{empty} (the former is possible if \( m \) is even and the latter if \( m \) is odd), then the type of \( G \) is defined by

\[
\Psi_m \land \bigwedge_{i=1}^{m} T_i \land \forall x (\Phi_{m+1}(x) \land \Phi_{m}(x)).
\]

Indeed, \( \Psi_m \land \bigwedge_{i=1}^{m} T_i \) is true on a graph \( H \) if and only if \( H \) has the \( m \)-tail type \((t_0, t_1, \ldots, t_m)\) and \( \text{rk} \, H \geq m+1 \). Let \( Q \subset V(H) \) denote the set of vertices not in the
tail part. Then $Q$ induces a complete or an empty subgraph exactly when $H$ satisfies $\forall x(\Phi_{m+1}(x) \lor \Phi_m(x))$.

If the head type of $G$ is normal, then the type of $G$ is defined by

$$\Psi_m \land \bigwedge_{i=1}^{m} T_i \land \neg\Psi_{m+1} \land \neg\forall x(\Phi_{m+1}(x) \lor \Phi_m(x)).$$

This definition ensures the rank of a graph to be exactly $m + 1$ and excludes the head types complete and empty.

### 7.2. A collapse theorem

**Theorem 7.3.** If a class of uncolored graphs is definable by a first-order formula with two variables, then it is definable by a first-order formula with two variables and one quantifier alternation.

The theorem easily follows from Lemmas 7.1 and 7.2. Let $C$ be a class of graphs definable by a formula with two variables of quantifier depth less than $m$. By Lemma 7.1, $C$ is the union of finitely many classes of graphs of the same type (each of rank at most $m$) and finitely many classes of graphs of the same $m$-tail type. By Lemma 7.2, $C$ is therefore definable by a first-order formula with two variables and one quantifier alternation. The proof is complete.

We conclude this section with several observations.

**Remark 7.4.** Part 1 of Lemma 7.1 and part 2 of Lemma 7.1 readily imply that two uncolored graphs are indistinguishable in $\text{FO}^2$ if and only if they have the same type. The type of a given graph $G$ can be determined in $\text{NC}^1$. This follows from two observations:

— Suppose that $v$ is in the kernel of $G$ while $u$ and $w$ are not, i.e., $\text{rk } v = \text{rk } G$ and $\text{rk } u, \text{rk } w < \text{rk } G$. If $u$ is of universal type and $w$ is of isolated type, then $\text{deg } w < \text{deg } v < \text{deg } u$.

— The degree of a vertex of isolated type increases together with its rank, while the degree of a vertex of universal type decreases as its rank increases.

Based on these observations, the type of $G$ is easy to determine after computing all vertex degrees. It follows that the equivalence problem for $\text{FO}^2$ over uncolored graphs is in $\text{NC}^1$. If extended to $\text{FO}^3$ or to colored graphs, the equivalence problem is known to be P-complete [Grohe 1999].

**Remark 7.5.** The $\text{FO}^2$-equivalence relation over trees degenerates to four classes whose representatives are, respectively, the path graphs $P_1$, $P_2$, $P_3$, and $P_4$. Here $P_n$ denotes the path on $n$ vertices. Note that $P_1$ is the single-vertex graph, $P_2$ is complete, $P_3$ is normal, and $P_3$ has rank 2. The equivalence classes of $P_1$ and $P_2$ are singletons. The equivalence class of $P_3$ consists of the stars with at least 3 vertices. The class of $P_3$ consists of all remaining trees, which are normal. As it is easy to see, any two inequivalent trees are distinguishable by a $\text{FO}^2$ formula with no quantifier alternation. This justifies the equality in the 1-st row of Figure 1.

**Remark 7.6.** In general, Theorem 7.3 is optimal with respect to the alternation number. Let $n \geq 5$ and consider the cycle $C_n$ on $n$ vertices and the wheel graph $W_n$ consisting of the cycle $C_{n-1}$ and a universal vertex. Since $\text{rk } C_n = 1$ and $\text{rk } W_n = 2$, these graphs are distinguishable in $\text{FO}^3$. However, if Spoiler plays only in $C_n$, Duplicator wins by moving in the $C_{n-1}$ subgraph of $W_n$, which is a normal graph. If Spoiler plays only in $W_n$, Duplicator wins because $C_n$ is normal. This example justifies the equality in the 6-th row of Figure 1.
8. DISCUSSION AND FURTHER QUESTIONS

We left several questions open. Is the logarithmic lower bound for $A^2(n)$ of Theorem 3.1 tight over trees? Furthermore, some of our arguments for $FO^2$ seem not to have obvious extensions to the larger number of variables. Can the logarithmic lower bound for $A^3(n)$ be improved over colored graphs, say, to a linear lower bound? How tight is the upper bound $D_{\Sigma}^{k}(G, H) \leq (v(G)v(H))^{k-1} + 1$ (cf. Theorem 6.1) if $k \geq 3$?

Is there a trade-off between the number of variables and the number of alternations? Specifically, suppose that $n$-element structures $G$ and $H$ are distinguishable in $FO^2$. In other terms, we know that $A^2(G, H)$ is finite, though it can be linear by Theorem 4.1. Does there exist a constant $k$ such that $A^k(G, H) = O(\log n)$ for any such $G$ and $H$? Similarly, can we reduce even the quantifier depth $D^k(G, H)$ if we take a larger $k$? A negative result in this direction is obtained by Immerman [1981] who constructed pairs of colored digraphs $G$ and $H$ such that $D^3(G, H) < \infty$ while $D^{FO}(G, H) > 2^{\log n - 1}$.

Is there a trade-off between the number of alternations and the quantifier depth? Specifically, let $D_a^k(G, H) = D_{\Sigma_k+1 \cup \Pi_k+1}^k(G, H)$. Suppose that $D_3^{2}(G, H) < \infty$. By Theorem 5.1 we know that this can require quadratic quantifier depth, that is, sometimes we can have $D_2^2(G, H) = \Omega(n^2)$. Is there a constant $a$ such that $D_a^k(G, H) = O(n)$ for all such $G$ and $H$?

Let $D^k_0(G)$ denote the minimum quantifier depth of a formula in $(\Sigma_{k+1} \cup \Pi_{k+1}) \cap FO^k$ defining a graph $G$ up to isomorphism. Note that $D^k_0(G) = \max_H D^k_0(G, H)$, where the maximum is taken over all graphs non-isomorphic to $G$. Theorem 5.4 shows examples of a large gap between the parameters $D^k_0(G, H)$ and $D^k_{a+1}(G, H)$. How far apart can the parameters $D^k_0(G)$ and $D^k_{a+1}(G)$ be from one another? If we consider the similar parameters for the unbounded-variable logic FO, then it is known [Pikhurko et al. 2006] that the gap between $D_3(G)$ and $D_0(G)$ can be huge: there is no total recursive function such that $D_0(G) \leq f(D_3(G))$.

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REFERENCES


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