

An optimal Gaifman normal form construction for structures of bounded degree

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Abstract—This paper’s main result presents a 3-fold exponential algorithm that transforms a first-order formula φ together with a number d into a formula in Gaifman normal form that is equivalent to φ on the class of structures of degree at most d . For structures of polynomial growth, we even get a 2-fold exponential algorithm.

These results are complemented by matching lower bounds: We show that for structures of degree 2, a 2-fold exponential blow-up in the size of formulas cannot be avoided. And for structures of degree 3, a 3-fold exponential blow-up is unavoidable.

As a result of independent interest we obtain a 1-fold exponential algorithm which transforms a given first-order sentence φ of a very restricted shape into a sentence in Gaifman normal form that is equivalent to φ on all structures.

Keywords—model theory; computational logic; first-order logic; Gaifman’s locality theorem; structures of bounded degree

I. INTRODUCTION

The intuition that first-order logic can only express local properties is formalized by the theorems by Hanf, by Gaifman, and by Schwentick and Barthelmann [8], [12], [15], [21]. All these results give normal forms for first-order formulas. In particular, formulas in Hanf normal form are Boolean combinations of statements of the form “there are at least k elements x whose r -neighborhood has isomorphism type τ ”. Formulas in Gaifman normal form are Boolean combinations of expressions of the form “there are at least k elements x of pairwise distance $> 2r$ whose r -neighborhood satisfies a formula $\varrho(x)$ ”.

Hanf’s and Gaifman’s theorem have found various applications in algorithms and complexity (cf., [4], [6], [10], [14], [17], [18], [22]). In particular, there are very general algorithmic meta-theorems stating that first-order model checking is fixed-parameter tractable for various classes of structures, and that first-order definable optimisation problems on such classes have polynomial time approximation schemes. In the context of such algorithms, questions about the efficiency of the normal forms have recently attracted interest [2], [5], [6], [13], [14], [20].

The first primitive-recursive algorithm for computing a Hanf normal form can be found in [6], [20]. The algorithm from [6], at first sight, seems to be non-elementary, but it actually is 4-fold exponential [3]. Finally, [2] presents a 3-fold exponential algorithm and proves a matching lower bound.

A striking difference between Hanf’s and Gaifman’s theorem is that the former only applies to structures of bounded degree, while the latter applies to all relational structures. Already Gaifman’s article [12] provides an algorithm for transforming formulas into Gaifman normal form. Dawar, Grohe, Kreutzer, and Schweikardt [5] proved that such a transformation is only possible at non-elementary cost, if the algorithm has to handle arbitrary first-order formulas and has to return a Gaifman normal form that is equivalent to the input formula on all structures (even, on all finite trees). But there is hope for more efficient algorithms if the input formula is of a restricted form or if the output formula has to be equivalent to the input formula only on a restricted class of structures.

Towards restricted formulas, we know from [14] that purely existential formulas can be transformed in 1-fold exponential time into *asymmetric* Gaifman normal form, a slightly weaker variant of Gaifman normal form.

Towards restricted structures, [5] observes that for every formula φ and every natural number d , there exists a formula in Gaifman normal form of 4-fold exponential size that is equivalent to φ on all structures of degree $\leq d$. Their proof, however, is a variant of the model theoretic proof of Gaifman’s theorem presented in [7], and it does not lead to a primitive recursive algorithm. The first author’s master’s thesis [16] provides an elementary (in fact, 5-fold exponential) procedure.

This paper’s main contribution gives a complete answer to the question of how difficult it is to transform formulas into equivalent Gaifman normal forms on structures of bounded degree: We present a 3-fold exponential algorithm and a matching lower bound. When restricting attention to structures whose r -neighborhoods are of size polynomial in r (e.g., structures of degree ≤ 2), our algorithm is 2-fold exponential, and this is also complemented by a matching lower bound.

As a result of independent interest, we obtain a 1-fold exponential algorithm that transforms an input sentence φ of a very restricted form into a Gaifman normal form sentence that is equivalent to φ on all structures. This contributes towards the following lines of Frick and Grohe [10]:

“As we mentioned, one of the main factors contributing to the heavy dependence of the running time of our algorithms on the size of the formula is the transformation into a “local formula” according to Gaifman’s theorem. [...] We do expect this complex-

ity to be nonelementary, but this does not rule out the existence of more efficient algorithms for particular classes of formulas [...] In general, we consider it as one of the main challenges for further research to reduce the dependence on the formula size [...].”

While our lower bound proofs are similar to the according proofs in [5], our upper bound provides a new method for constructing Gaifman normal forms. We proceed as follows:

- (1) Restrict attention to sentences of the form
 - (*) : there are at least k elements x that satisfy $\varrho(x)$, where $\varrho(x)$ speaks only about the r -neighborhood around x and show that these can be transformed in 1-fold exponential time into an equivalent (on all structures) sentence in Gaifman normal form. The ingredient crucial for our proof is an analysis of the potential distributions of nodes of a particular color in a labeled graph. Cf., Section III-A and Theorem III.4.
- (2) For the 3-fold exponential Gaifman normal form algorithm for structures of bounded degree, we can then combine (1) with the 3-fold exponential Hanf normal form construction of [2]: First, transform an arbitrary given first-order sentence Φ into a Hanf normal form Φ^H equivalent to Φ on the class of all structures of degree at most d . Then, Φ^H is a Boolean combination of sentences of the form (*) which, according to (1), can be transformed into Gaifman normal form. A closer analysis of the properties of the algorithms of (1) and [2] then shows that the overall running time is still 3-fold exponential in the size of the input formula Φ . A small additional observation also allows us to handle arbitrary formulas Φ rather than just sentences. Cf., Sections III-B, III-C and Theorem III.1.

The rest of the paper is structured as follows: Section II fixes the notations used throughout the paper, Section III provides algorithms for transforming formulas into Gaifman normal form, and Section IV proves matching lower bounds. Due to space limitations, some technical details of our proofs are deferred to the full version of this paper.

II. PRELIMINARIES

We write \mathbb{N} to denote the set of non-negative integers, and we let $\mathbb{N}_{\geq 1} := \mathbb{N} \setminus \{0\}$. The set of non-negative real numbers is denoted $\mathbb{R}_{\geq 0}$. For $r > 0$ we write $\log(r)$ to denote the logarithm of r with respect to base 2. If f is a function from \mathbb{N} to $\mathbb{R}_{\geq 0}$, then $\text{poly}(f(n))$ denotes the class of all functions $g: \mathbb{N} \rightarrow \mathbb{R}_{\geq 0}$ for which there exists a number $c > 0$ such that for all sufficiently large $n \in \mathbb{N}$ we have $g(n) \leq (f(n))^c$.

A. Structures and formulas

A signature σ is a finite set of relation and constant symbols. Associated with every relation symbol R is a positive integer $\text{ar}(R)$ called the *arity* of R . The *size* $|\sigma|$ of σ is the number of its constant symbols plus the sum of the arities of its relation

symbols. The signature σ is called *relational* if it does not contain any constant symbol.

A σ -structure \mathcal{A} consists of a non-empty set A called the *universe* of \mathcal{A} , a relation $R^{\mathcal{A}} \subseteq A^{\text{ar}(R)}$ for each relation symbol $R \in \sigma$, and an element $c^{\mathcal{A}} \in A$ for each constant symbol $c \in \sigma$.

We use the standard notation concerning first-order formulas, cf. [7], [19]. In particular, $\text{FO}(\sigma)$ denotes the class of all first-order formulas of signature σ , and $\text{qr}(\varphi)$ denotes the quantifier rank of an $\text{FO}(\sigma)$ -formula φ . We write $\text{free}(\varphi)$ to denote the set of free variables of φ , and we often write $\varphi(\bar{x})$, for $\bar{x} = (x_1, \dots, x_n)$ with $n \geq 0$, to indicate that $\text{free}(\varphi)$ is a subset of $\{x_i : 1 \leq i \leq n\}$.

For a class \mathfrak{C} of structures, we say that two $\text{FO}(\sigma)$ -formulas $\varphi(\bar{x})$ and $\psi(\bar{x})$ are *equivalent on \mathfrak{C}* if for all σ -structures $\mathcal{A} \in \mathfrak{C}$ and all $\bar{a} \in A^n$ we have $\mathcal{A} \models \varphi[\bar{a}]$ iff $\mathcal{A} \models \psi[\bar{a}]$.

The length (or, size) $\|\varphi\|$ of an $\text{FO}(\sigma)$ -formula φ is its length when viewed as a word over the alphabet $\sigma \cup \{=\} \cup \{\exists, \forall, \neg, \wedge, \vee, \rightarrow, \leftrightarrow, (,)\} \cup \{, \} \cup \text{Var}$, where Var is a countable set of variable symbols.

For a number $k \geq 1$ and a formula $\varphi(\bar{x}, y)$ we write

$$\exists^{\geq k} y \varphi(\bar{x}, y)$$

as a shorthand for the formula

$$\exists y_1 \cdots \exists y_k \left(\bigwedge_{1 \leq i < j \leq k} \neg y_i = y_j \wedge \forall y \left(\bigvee_{1 \leq i \leq k} y = y_i \rightarrow \varphi(\bar{x}, y) \right) \right).$$

Note that, given k, y , and φ , this formula can be constructed in time $O(k^2 + \|\varphi\|)$.

B. Gaifman normal form

For a σ -structure \mathcal{A} , we write $G_{\mathcal{A}}$ to denote the Gaifman graph of \mathcal{A} , i.e., the undirected, loop-free graph with vertex set A and an edge between two distinct vertices $a, b \in A$ iff there exists an $R \in \sigma$ and a tuple $(a_1, \dots, a_{\text{ar}(R)}) \in R^{\mathcal{A}}$ such that $a, b \in \{a_1, \dots, a_{\text{ar}(R)}\}$.

The *distance* $\text{dist}^{\mathcal{A}}(a, b)$ between two elements $a, b \in A$ in a σ -structure \mathcal{A} is the minimal length (i.e., the number of edges) of a path from a to b in the Gaifman graph $G_{\mathcal{A}}$.

For $r \geq 0$ and $a \in A$, the r -neighborhood of a in \mathcal{A} is the set $N_r^{\mathcal{A}}(a) = \{b \in A : \text{dist}^{\mathcal{A}}(a, b) \leq r\}$. The r -neighborhood of a set $W \subseteq A$ is the set $N_r^{\mathcal{A}}(W) := \bigcup_{a \in W} N_r^{\mathcal{A}}(a)$. If $\bar{a} = (a_1, \dots, a_n)$, we write $N_r^{\mathcal{A}}(\bar{a})$ instead of $N_r^{\mathcal{A}}(\{a_1, \dots, a_n\})$.

For each $r \in \mathbb{N}$ there is an $\text{FO}(\sigma)$ -formula $\text{dist}_{\leq r}(x, y)$ of length $O(\log(r))$ expressing that the distance between x and y is at most r : The formulas $\text{dist}_{\leq 0}(x, y)$ and $\text{dist}_{\leq 1}(x, y)$ can be defined according to the edge relation of the Gaifman graph of σ -structures, and for $r \geq 1$ we can choose

$$\text{dist}_{\leq 2r}(x, y) := \exists u \forall z ((z = x \vee z = y) \rightarrow \text{dist}_{\leq r}(z, u)),$$

$$\text{dist}_{\leq 2r+1}(x, y) := \exists z (\text{dist}_{\leq 1}(x, z) \wedge \text{dist}_{\leq 2r}(z, y)).$$

We usually write $\text{dist}(x, y) \leq r$ instead of $\text{dist}_{\leq r}(x, y)$ and $\text{dist}(x, y) > r$ instead of $\neg \text{dist}_{\leq r}(x, y)$. Furthermore, if $\bar{x} = (x_1, \dots, x_n)$ is a sequence of $n \geq 1$ variables and y is another variable, then we write $\text{dist}(\bar{x}, y) \leq r$ to denote the formula $\bigvee_{i=1}^n \text{dist}(x_i, y) \leq r$.

An FO(σ)-formula $\varphi(\bar{x})$ is called *r-local around \bar{x}* if for all σ -structures \mathcal{A} and all $\bar{a} \in A^n$ we have $\mathcal{A} \models \varphi[\bar{a}]$ iff $\mathcal{A} \models \varphi^r[\bar{a}]$, where $\varphi^r(\bar{x})$ is the *r-relativisation* of $\varphi(\bar{x})$, i.e., the formula obtained from $\varphi(\bar{x})$ by replacing each subformula of the form $\exists z \psi$ by $\exists z (\text{dist}(\bar{x}, z) \leq r \wedge \psi)$ and each subformula of the form $\forall z \psi$ by $\forall z (\text{dist}(\bar{x}, z) \leq r \rightarrow \psi)$. Thus, *r-local formulas $\varphi(\bar{x})$* only speak about the *r-neighborhood* of \bar{x} . A formula $\varphi(\bar{x})$ is *local* if it is *r-local around \bar{x}* , for some $r \geq 0$.

A *basic local sentence* is an FO(σ)-sentence of the form

$$\exists x_1 \cdots \exists x_k \left(\bigwedge_{1 \leq i < j \leq k} \text{dist}(x_i, x_j) > 2r \wedge \bigwedge_{1 \leq i \leq k} \varphi(x_i) \right),$$

where $k, r \geq 1$ and $\varphi(x)$ is *r-local around x* .

A formula is in *Gaifman normal form* if it is a Boolean combination of local formulas and basic local sentences.

From Gaifman's famous theorem [12] we know an algorithm which transforms every FO(σ)-formula Ψ into an equivalent formula Ψ^G in Gaifman normal form. In [5] it was shown that there is no elementary bound on the length of Ψ^G in terms of the length of Ψ .

C. Bounded structures

The *degree* of a σ -structure \mathcal{A} is the degree of its Gaifman graph $G_{\mathcal{A}}$. Let $\nu: \mathbb{N} \rightarrow \mathbb{N}$ be a function. A σ -structure \mathcal{A} is *ν -bounded* if $|N_r^{\mathcal{A}}(a)| \leq \nu(r)$ for all $r \in \mathbb{N}$ and $a \in A$. Clearly, if \mathcal{A} is ν -bounded, then it has degree $\leq \nu(1)-1$. On the other hand, if \mathcal{A} has degree $\leq d$, then \mathcal{A} is ν_d -bounded for $\nu_d: \mathbb{N} \rightarrow \mathbb{N}$ with $\nu_d(r) = 1 + d \cdot \sum_{0 \leq i < r} (d-1)^i$. Thus, \mathcal{A} has degree $\leq d$ if, and only if, it is ν_d -bounded. Furthermore, \mathcal{A} is ν -bounded for some function ν if, and only if, \mathcal{A} is ν_d -bounded for some $d \in \mathbb{N}$. We will restrict attention to *strictly increasing* functions $\nu: \mathbb{N} \rightarrow \mathbb{N}$. This is reasonable, since then $(r+1)$ -neighborhoods may contain more elements than r -neighborhoods, and it excludes pathological cases where ν -boundedness of a structure implies that the structure is a disjoint union of finite structures whose size is bounded by a constant depending on ν .

Two FO(σ)-formulas Ψ and Ψ^* are called *ν -equivalent* if they are equivalent on the class of all ν -bounded σ -structures.

Let \mathcal{A} be a σ -structure, let $n \geq 1$ and let $\bar{a} = (a_1, \dots, a_n) \in A^n$. Let c_1, \dots, c_n be n distinct and new constant symbols. For $r \geq 1$, the *r-sphere around \bar{a}* is the $\sigma \cup \{c_1, \dots, c_n\}$ -structure

$$\mathcal{N}_r^{\mathcal{A}}(\bar{a}) := (\mathcal{A}_{|N_r^{\mathcal{A}}(\bar{a})}, \bar{a}),$$

where $\mathcal{A}_{|N_r^{\mathcal{A}}(\bar{a})}$ is the induced substructure of \mathcal{A} on $N_r^{\mathcal{A}}(\bar{a})$, and the constant symbols c_1, \dots, c_n are interpreted by the elements a_1, \dots, a_n .

An *r-sphere with n centers* is a $\sigma \cup \{c_1, \dots, c_n\}$ -structure $\tau = (B, \bar{b})$ with $\bar{b} = (b_1, \dots, b_n) \in B^n$ and $B = N_r^B(\bar{b})$. We say that τ is *realised by \bar{a} in \mathcal{A}* iff $\mathcal{N}_r^{\mathcal{A}}(\bar{a})$ is isomorphic to τ .

Note that a ν -bounded r -sphere τ with n centers contains at most $n \cdot \nu(r)$ elements. Thus, there is an FO(σ)-formula $\text{sph}_r(\bar{x})$ of size $\text{poly}(n\nu(r))$ such that for all σ -structures \mathcal{A} and all elements $\bar{a} = (a_1, \dots, a_n) \in A^n$ we have $\mathcal{A} \models \text{sph}_r[\bar{a}]$ iff τ is realised by \bar{a} in \mathcal{A} .

D. Hanf normal form

A *Hanf-formula* with free variables $\bar{x} = (x_1, \dots, x_n)$, for $n \geq 0$, is a formula of the form

$$\exists^{\geq k} y \text{sph}_{\tau}(\bar{x}, y)$$

where τ is the isomorphism type of a finite r -sphere (for an $r \in \mathbb{N}$) with $n+1$ centers. Hanf-formulas without free variables (i.e., $n = 0$) are called *Hanf-sentences*. A formula is in *Hanf normal form* if it is a Boolean combination of Hanf-formulas.

In [2], Bollig and Kuske presented a 3-fold exponential algorithm that transforms a given FO(σ)-formula into a ν_d -equivalent formula in Hanf normal form. In the slightly more general setting of ν -bounded structures, their proof yields the following (a proof will be included in the full version of this paper).

Theorem II.1 ([2]). *Fix a relational signature σ and a time-constructible strictly increasing function $\nu: \mathbb{N} \rightarrow \mathbb{N}$. There is an algorithm which transforms an input FO(σ)-formula Ψ of quantifier rank q in time*

$$2^{\text{poly}(\|\Psi\| \cdot \nu(4^q))} \quad (1)$$

into a ν -equivalent formula Ψ^H in Hanf normal form.

Moreover, each Hanf-formula occurring in Ψ^H is of the form $\exists^{\geq k} y \text{sph}_{\tau}(\bar{x}, y)$, where $k \leq \|\Psi\| \cdot (q+1) \cdot \nu(4^q)$, τ is a ν -bounded r -sphere of radius $r \leq 4^q$, and $|\bar{x}| \leq |\text{free}(\Psi)|$.

Furthermore, the degree of the polynomial in the expression (1) is linear in the size of the signature σ .

III. THE UPPER BOUND

Throughout this section we let σ be a fixed finite relational signature and we let $\nu: \mathbb{N} \rightarrow \mathbb{N}$ be a fixed time-constructible strictly increasing function. This section's main result is an elementary algorithm which transforms an input FO(σ)-formula Ψ into a ν -equivalent formula in Gaifman normal form. The precise statement of the result is as follows:

Theorem III.1. *Fix a relational signature σ and a time-constructible strictly increasing function $\nu: \mathbb{N} \rightarrow \mathbb{N}$. There is an algorithm which transforms an input FO(σ)-formula Ψ of quantifier rank q in time*

$$2^{\text{poly}(\|\Psi\| \cdot \nu(2 \cdot 4^q + 1))} \quad (2)$$

into a ν -equivalent formula Ψ^G in Gaifman normal form.

The degree of the polynomial in the expression (2) is linear in the size of the signature σ .

Thus, if ν is exponential, then Ψ can be transformed into Ψ^G in 3-fold exponential time — e.g., if $\nu = \nu_d$ for $d \geq 3$, in time $2^{d^{2^{O(\|\Psi\|)}}}$. If ν is polynomial, then the transformation requires only 2-fold exponential time, i.e. time $2^{2^{O(\|\Psi\|)}}$.

The remainder of Section III is devoted to the proof of Theorem III.1. The first step of our algorithm uses Theorem II.1 to transform Ψ into a ν -equivalent formula Ψ^H in Hanf normal form. Afterwards, we transform each Hanf-formula occurring in Ψ^H into a ν -equivalent formula in Gaifman

normal form. The details of this transformation are explained in the next subsections — first for the case of Hanf-sentences, and afterwards for the case of Hanf-formulas that contain free variables.

A. Transforming Hanf-sentences into Gaifman normal form

In this subsection we in fact show a more general result that

- does not restrict attention to ν -equivalence, but establishes equivalence with respect to the class of *all* σ -structures, and
- does not restrict attention to Hanf-sentences, but considers formulas of the form $\exists^{\geq k} y \varrho(y)$, where $\varrho(y)$ is an arbitrary FO(σ)-formula that is r -local around y .

For a σ -structure \mathcal{A} , we consider the nodes a of its Gaifman graph $G_{\mathcal{A}}$ to be colored either red or blue, depending on whether or not $\mathcal{A} \models \varrho[a]$. When evaluated in \mathcal{A} , the formula $\Psi := \exists^{\geq k} y \varrho(y)$ then states that $G_{\mathcal{A}}$ has at least k red nodes.

The following lemma tells us about the distribution of red nodes. This provides information that will be useful for constructing a Gaifman normal form sentence equivalent to Ψ .

Lemma III.2. *Let $k, r, c \in \mathbb{N}_{\geq 1}$. For every graph $G = (V, E)$ and every mapping $\gamma: V \rightarrow \{\text{red}, \text{blue}\}$, one of the following statements is true:*

- There is no red node in (G, γ) .*
- (G, γ) has at least k red nodes of pairwise distance $> cr$.*
- There is a unique $\ell \in \{1, \dots, k-1\}$ such that (G, γ) contains ℓ , but not $\ell+1$ red nodes of pairwise distance $> cr$. There exists a set W of red nodes of size $|W| \in \{1, \dots, \ell\}$ such that for $s := \ell - |W|$ and $R_s := (c+1)^s \cdot cr$ the following is true:*
 - $\text{dist}(a, b) > cR_s$, for all $a, b \in W$ with $a \neq b$, and*
 - every red node of (G, γ) belongs to $N_{R_s}(W)$.*

Proof: It suffices to consider the case where neither (a) nor (b) is true. Our goal is to show that in this case (c) holds.

Since neither (a) nor (b) is true, there is an $\ell \in \{1, \dots, k-1\}$ such that (G, γ) contains ℓ , but not $\ell+1$ red nodes of pairwise distance $> cr$.

For $j \geq 0$ let $R_j := (c+1)^j \cdot cr$. We construct a sequence of finite sets W_j of size $\ell - j$, such that $W_0 \supset W_1 \supset W_2 \supset \dots$, and for every $j \geq 0$ every red node of (G, γ) belongs to $N_{R_j}(W_j)$.

Let W_0 be a set of ℓ red nodes of pairwise distance $> cr$. Then, $N_{cr}(W_0)$ contains *all* red nodes of (G, γ) (otherwise we could extend W_0 , contradicting our choice of ℓ).

Let the sets W_0, \dots, W_j be already constructed for some $j \geq 0$. If all elements of W_j have pairwise distance $> cR_j$, then we let $W := W_j$ and terminate the construction. Otherwise, let a and b be elements in W_j with $\text{dist}(a, b) \leq cR_j$. We let $W_{j+1} := W_j \setminus \{b\}$. Note that $N_{R_j}(b) \subseteq N_{(c+1)R_j}(a)$. Since $R_{j+1} = (c+1)R_j$, we thus know that every red node of (G, γ) belongs to the R_{j+1} -neighborhood of W_{j+1} .

Since $|W_j| = \ell - j$, the construction ends after at most $\ell - 1$ steps, resulting with a set W with the desired properties. ■

Let us mention that results similar to Lemma III.2 have been used before, cf. e.g. Claim 4.4 in [1] and Lemma 8 in [4].

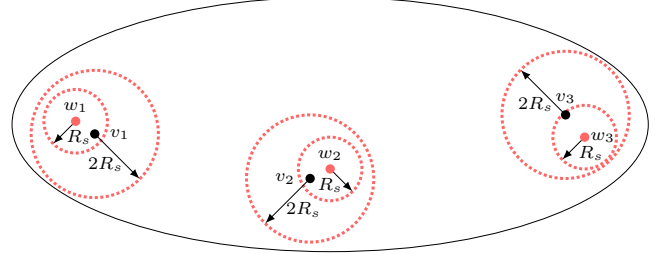


Fig. 1. Illustration for Lemma III.3 for $\ell - s = 3$. All red nodes of (G, γ) belong to the R_s -neighborhood of the w_i , and thus to the $2R_s$ -neighborhood of the v_i , for $i \in \{1, 2, 3\}$. The w_i have pairwise distance $> 8R_s$.

We can use Lemma III.2 to show the following technical result, which is the key lemma that enables us to find an appropriate sentence in Gaifman normal form that is equivalent to the sentence $\Psi = \exists^{\geq k} y \varrho(y)$.

Lemma III.3. *Let $k, r \in \mathbb{N}_{\geq 1}$, let $G = (V, E)$ be a graph, and let $\gamma: V \rightarrow \{\text{red}, \text{blue}\}$. For $s \in \mathbb{N}$ let $R_s := 9^s 8r$.*

(G, γ) has at least k red nodes if, and only if, one of the following statements is true:

- (G, γ) has at least k red nodes of pairwise distance $> 8r$.*
- (G, γ) has a red node whose R_k -neighborhood contains at least k red nodes.*
- Each of the following statements is true:*
 - There is a unique $\ell \in \{1, \dots, k-1\}$ such that (G, γ) contains ℓ , but not $\ell+1$ red nodes of pairwise distance $> 8r$.*
 - There is a unique $s \in \{0, \dots, \ell-1\}$ such that there exist $\ell-s$ red nodes of pairwise distance $> 8R_s$ and either $s = 0$ or there do not exist $\ell-(s-1)$ red nodes of pairwise distance $> 8R_{s-1}$.*
 - There is a number t with $1 \leq t \leq \ell-s$ and there are numbers $1 \leq n_1 < \dots < n_t < k$ and $m_1, \dots, m_t \in \{1, \dots, k\}$ such that $m_1 + \dots + m_t = \ell-s$ and $m_1 n_1 + \dots + m_t n_t \geq k$.*
 - For each $j \in \{1, \dots, t\}$ there are at least m_j red nodes x of pairwise distance $> 6R_s$ such that $N_{2R_s}(x)$ contains exactly n_j red nodes.*

Proof: “ \implies ”: Let (G, γ) contain at least k red nodes. It suffices to consider the case where neither (1) nor (2) is true. Our goal is to show that in this case (3) is satisfied.

We use Lemma III.2 for $c = 8$. Note that (G, γ) neither satisfies item (a) nor item (b) of Lemma III.2. Thus, item (c) of Lemma III.2 must be true. In particular there is an $\ell \in \{1, \dots, k-1\}$ such that (G, γ) contains ℓ , but not $\ell+1$ red nodes of pairwise distance $> 8r$, and hence (3i) is satisfied.

Let $s \in \{0, \dots, \ell-1\}$ be minimal such that there exists a set $W = \{w_1, \dots, w_{\ell-s}\}$ of $\ell-s$ red nodes of pairwise distance $> 8R_s$ where $N_{R_s}(W)$ contains all red nodes of (G, γ) — such a number exists by Lemma III.2(c). In particular, (3ii) is satisfied.

For every $i \in \{1, \dots, \ell-s\}$ let n_i be the number of red nodes in $N_{R_s}(w_i)$. Since, by assumption, (2) does not hold,

we know that $1 \leq n_i < k$. In summary, we now know the following (see Figure 1 for an illustration):

- $\text{dist}(w_i, w_j) > 8R_s$, for all $i, j \in \{1, \dots, \ell-s\}$ with $i \neq j$.
- Every red node of (G, γ) belongs to $N_{R_s}(\{w_1, \dots, w_{\ell-s}\})$. Since, by assumption, (G, γ) contains at least k red nodes, we know that $n_1 + \dots + n_{\ell-s} \geq k$.
- For all $v_i \in N_{R_s}(w_i)$ and $v_j \in N_{R_s}(w_j)$ with $i \neq j$ we have $\text{dist}(v_i, v_j) > 6R_s$.
- For every $v_i \in N_{R_s}(w_i)$, the set $N_{2R_s}(v_i)$ contains exactly the same red nodes as $N_{R_s}(w_i)$.

Let us now group the numbers $n_1, \dots, n_{\ell-s}$ according to their size. Let $t := |\{n_1, \dots, n_{\ell-s}\}|$ be the number of distinct sizes, and choose $i_1, \dots, i_t \in \{1, \dots, \ell-s\}$, such that $\{n_1, \dots, n_{\ell-s}\} = \{n_{i_1}, \dots, n_{i_t}\}$. Furthermore, let $m_{i_j} := |\{i \in \{1, \dots, \ell-s\} : n_i = n_{i_j}\}|$ be the number of occurrences of the value n_{i_j} . Then, the following is true:

- $m_{i_1} + \dots + m_{i_t} = \ell-s$ and $m_{i_1}n_{i_1} + \dots + m_{i_t}n_{i_t} = n_1 + \dots + n_{\ell-s} \geq k$.
- For every $j \in \{1, \dots, t\}$ the following is true: There are at least m_{i_j} red nodes x of pairwise distance $> 6R_s$ such that $N_{2R_s}(x)$ contains exactly n_{i_j} red nodes.

Thus, items (3iii) and (3iv) are satisfied. This completes the proof of “ \Rightarrow ”.

“ \Leftarrow ”: If (1) or (2) is true, then (G, γ) obviously contains at least k red nodes.

If (3) is satisfied, then according to (3i) there are ℓ but not $\ell+1$ red nodes of pairwise distance $> 8r$.

According to (3ii), there are red nodes $w_1, \dots, w_{\ell-s}$ of pairwise distance $> 8R_s$, for which the following is true:

- (A) All red nodes of (G, γ) belong to $N_{R_s}(\{w_1, \dots, w_{\ell-s}\})$.

(Assume there is a red node $y \notin N_{R_s}(\{w_1, \dots, w_{\ell-s}\})$. If $s = 0$, then the $\ell+1$ red nodes w_1, \dots, w_ℓ, y have pairwise distance $> 8r$, contradicting (3i). In case that $s > 0$ we know that $\text{dist}(y, w_i) > R_s = 9R_{s-1} > 8R_{s-1}$, for all $i \in \{1, \dots, \ell-s\}$. Thus, there are $\ell-(s-1)$ red nodes of pairwise distance $> 8R_{s-1}$. This contradicts the choice of s according to (3ii).)

- (B) For all nodes $v_i \in N_{R_s}(w_i)$ and $v_j \in N_{R_s}(w_j)$ with $i \neq j$, we have $\text{dist}(v_i, v_j) > 6R_s$.

(This is obvious, since $\text{dist}(w_i, w_j) > 8R_s$.)

- (C) For every $i \in \{1, \dots, \ell-s\}$ and every node $v_i \in N_{R_s}(w_i)$, the following is true: $N_{2R_s}(v_i)$ contains exactly the same red nodes as $N_{R_s}(w_i)$.

(This is an immediate consequence of (A) and (B).)

From (3iv) we know that for every $j \in \{1, \dots, t\}$ there are red nodes $x_{j,1}, \dots, x_{j,m_j}$ of pairwise distance $> 6R_s$, such that for each $i \in \{1, \dots, m_j\}$ the set $N_{2R_s}(x_{j,i})$ contains exactly n_j red nodes. Due to (A), for any $x_{j,i}$ there exists a $k_{j,i} \in \{1, \dots, \ell-s\}$ such that $x_{j,i} \in N_{R_s}(w_{k_{j,i}})$. Furthermore, the following must be true:

- (D) For all $j, j' \leq t$, $i \leq m_j$, and $i' \leq m_{j'}$ with $k_{j,i} = k_{j',i'} =: \kappa$, we have $(j, i) = (j', i')$.

(Since the nodes $x_{j,i}$ and $x_{j',i'}$ both belong to $N_{R_s}(w_\kappa)$, their distance is $\leq 2R_s$. From (C) we know that $N_{2R_s}(x_{j,i})$ contains exactly the same red nodes as $N_{2R_s}(x_{j',i'})$. Thus, $n_j = n_{j'}$, and hence $j = j'$. Consequently $i = i'$, for otherwise the distance of $x_{j,i}$ and $x_{j,i'}$ would be $> 6R_s$.)

(D) implies that each of the $x_{j,i}$ belongs to the neighborhood of a different element from $\{w_1, \dots, w_{\ell-s}\}$. With (3iv) we thus obtain that there are $m_1n_1 + \dots + m_tn_t$ distinct red nodes. According to (3iii), this number is $\geq k$.

Thus we have shown that (G, γ) has at least k red nodes. This completes the proof of “ \Leftarrow ” and the proof of Lemma III.3. ■

We are now ready to prove this subsection’s main result.

Theorem III.4. *Let σ be a fixed relational signature. Let $k, r \geq 1$, let $\varrho(y)$ be an $\text{FO}(\sigma)$ -formula that is r -local around y , and let $\Psi := \exists^{\geq k} y \varrho(y)$. Then Ψ is equivalent, on the class of all σ -structures, to a sentence Ψ^G in Gaifman normal form of size $2^{O(k \log(k))} (\log(r) + \|\varrho\|)$.*

Furthermore, there is an algorithm which, on input (k, r, ϱ) , constructs Ψ^G in time $2^{O(k \log(k))} (\log(r) + \|\varrho\|)$.

Proof: The formula Ψ^G is obtained by a direct translation of the statement of Lemma III.3 into a Boolean combination of basic local sentences. To estimate the time needed for performing this construction, we explicitly spell out the translation. For this, the following notation will be useful.

Let $n, k, r \geq 1$ and $R \geq r$, and let $\varphi(y)$ be a formula that is r -local around y . Then $\chi_R^k(\varphi) :=$

$$\exists x_1 \dots \exists x_k \left(\bigwedge_{1 \leq i < j \leq k} \text{dist}(x_i, x_j) > 2R \wedge \bigwedge_{1 \leq i \leq k} \varphi(x_i) \right)$$

is a basic local sentence of size $O(k^2 \log(R) + k\|\varphi\|)$. Furthermore

$$\lambda_R^n(x) := \varrho(x) \wedge \exists^{\geq n} y (\text{dist}(x, y) \leq R \wedge \varrho(y)) \quad \text{and}$$

$$\lambda_R^{\leq n}(x) := \lambda_R^n(x) \wedge \neg \lambda_R^{n+1}(x)$$

are formulas of size $O(n^2 + \log(R) + \|\varrho\|)$ that are $(R+r)$ -local around x .

We now let $\Psi^G := \Psi_{(1)}^G \vee \Psi_{(2)}^G \vee \Psi_{(3)}^G$ where, for each $j \in \{1, 2, 3\}$, $\Psi_{(j)}^G$ is a formalisation of statement (j) of Lemma III.3. I.e., for $R_s := 9^s 8r$ (for $s \in \mathbb{N}$), $\Psi_{(1)}^G := \chi_{4r}^k(\varrho)$ and $\Psi_{(2)}^G := \exists x \lambda_{R_k}^k(x)$. Note that both formulas are basic local sentences of size $O(k^2 \log(R_k) + k\|\varrho\|)$. The formula $\Psi_{(3)}^G$ is chosen as follows:

$$\Psi_{(3)}^G := \bigvee_{\substack{1 \leq \ell < k \\ 0 \leq s < \ell}} \left(\chi_{4r}^\ell(\varrho) \wedge \neg \chi_{4r}^{\ell+1}(\varrho) \wedge \vartheta_{\ell,s} \wedge \xi_{\ell,s} \right),$$

where

$$\begin{aligned}\vartheta_{\ell,0} &:= \chi_{4R_0}^\ell(\varrho) & \text{and, for } s \geq 1: \\ \vartheta_{\ell,s} &:= \chi_{4R_s}^{\ell-s}(\varrho) \wedge \neg \chi_{4R_{s-1}}^{\ell-(s-1)}(\varrho) & \text{and, for } s \geq 0: \\ \xi_{\ell,s} &:= \bigvee_{t=1}^{\ell-s} \bigvee_{D_{\ell,s,t}} \bigwedge_{j=1}^t \chi_{3R_s}^{m_j}(\lambda_{2R_s}^{\overline{n_j}}(x)),\end{aligned}$$

where “ $\bigvee_{D_{\ell,s,t}}$ ” is the disjunction over all possible choices of numbers $n_1, \dots, n_t, m_1, \dots, m_t \in \{1, \dots, k\}$ such that $1 \leq n_1 < \dots < n_t < k$, $m_1 + \dots + m_t = \ell - s$, and $m_1 n_1 + \dots + m_t n_t \geq k$.

Note that the formula $\lambda_{2R_s}^{\overline{n_j}}(x)$ is $(2R_s + r)$ -local and thus $3R_s$ -local around x . Hence, $\chi_{3R_s}^{m_j}(\lambda_{2R_s}^{\overline{n_j}}(x))$ is a basic local sentence.

Also, the other $\chi_b^a(\varrho)$ -formulas (with $a \in \{\ell, \ell+1, \ell-s, \ell-(s-1)\}$ and $b \in \{4r, 4R_s, 4R_{s-1}\}$) that $\Psi_{(3)}^G$ is built of, are basic local sentences.

Thus, Ψ^G is a sentence in Gaifman normal form which, due to Lemma III.3 is equivalent to Ψ (on all σ -structures).

It remains to estimate the size of Ψ^G :

- The size of $\vartheta_{\ell,s}$ and $(\chi_{4r}^\ell(\varrho) \wedge \neg \chi_{4r}^{\ell+1}(\varrho) \wedge \vartheta_{\ell,s})$ is $O(k^2 \log(R_k) + k||\varrho||)$.
- The size of $\chi_{3R_s}^{m_j}(\lambda_{2R_s}^{\overline{n_j}}(x))$ is $O(k^3 \log(R_k) + k||\varrho||)$.
- The size of $\xi_{\ell,s}$ is $O(k \cdot k^{2k} \cdot k \cdot ||\chi_{3R_s}^{m_j}(\lambda_{2R_s}^{\overline{n_j}}(x))||)$,
i.e., $||\xi_{\ell,s}|| = O(k^{2k+5} \log(R_k) + k^{2k+3}||\varrho||)$.
- The size of $\Psi_{(3)}^G$ is $O(k^2 \cdot (k^{2k+5} \log(R_k) + k^{2k+3}||\varrho||))$,
i.e., $||\Psi_{(3)}^G|| = O(k^{2k+7} \log(R_k) + k^{2k+5}||\varrho||)$.
- Thus, also Ψ^G is of size $O(k^{2k+7} \log(R_k) + k^{2k+5}||\varrho||)$.

Since $R_k = 9^k 8r$, we obtain that $||\Psi^G|| =$

$$O(k^{2k+8} \log(r) + k^{2k+5}||\varrho||) \subseteq 2^{O(k \log(k))} (\log(r) + ||\varrho||).$$

Furthermore, there obviously is an algorithm which, on input (k, r, ϱ) , constructs Ψ^G in time $2^{O(k \log(k))} (\log(r) + ||\varrho||)$. This completes the proof of Theorem III.4. \blacksquare

Remark III.5. In the particular case that $\varrho(y)$ is of the form $\text{sph}_\tau(y)$, for a ν -bounded r -sphere τ with a single center, we get the transformation of a Hanf-sentence into an equivalent sentence in Gaifman normal form:

Recall from Section II that $\text{sph}_\tau(y)$ is of size $\text{poly}(\nu(r))$ and ν is strictly increasing. Thus, from Theorem III.4 we obtain an algorithm which, on input $(k, r, \text{sph}_\tau(y))$, computes in time $2^{O(k \log k)} \cdot \text{poly}(\nu(r))$ a Gaifman normal form sentence equivalent to $\exists^{\geq k} y \text{sph}_\tau(y)$.

B. Transforming Hanf-formulas into Gaifman normal form

In this subsection we show how to transform Hanf-formulas with $n \geq 1$ free variables $\bar{x} = (x_1, \dots, x_n)$ into ν -equivalent formulas in Gaifman normal form. For performing this transformation, we will use Remark III.5.

This subsection's main result reads as follows:

Theorem III.6. Let σ be a fixed relational signature and let $\nu: \mathbb{N} \rightarrow \mathbb{N}$ be a time-constructible strictly increasing function. Let $k, r, n \geq 1$ and let τ be a ν -bounded r -sphere with $n+1$ centers. Let $\bar{x} := (x_1, \dots, x_n)$ and let $\Psi(\bar{x}) := \exists^{\geq k} y \text{sph}_\tau(\bar{x}, y)$. Then $\Psi(\bar{x})$ is ν -equivalent to a formula $\Psi^G(\bar{x})$ in Gaifman normal form of size $2^{\text{poly}(k + n\nu(2r+1))}$.

Furthermore, there is an algorithm which, on input $(k, r, \text{sph}_\tau(\bar{x}, y))$ computes $\Psi^G(\bar{x})$ in time $2^{\text{poly}(k + n\nu(2r+1))}$.

Proof: Recall from Section II that the formula $\text{sph}_\tau(\bar{x}, y)$ has size $\text{poly}(n\nu(r))$. The formula $\text{sph}_\tau(\bar{x}, y)$ contains a complete description of the isomorphism type of τ . Thus, in time $\text{poly}(|\text{sph}_\tau(\bar{x}, y)|)$ we can decide whether τ stipulates

Case 1: $y \in N_{2r+1}(\{x_1, \dots, x_n\})$ or

Case 2: $\text{dist}(x_i, y) > 2r+1$, for all $i \in \{1, \dots, n\}$.

Case 1 can be handled easily, since in this case the formula $\Psi(\bar{x})$ is equivalent to the formula

$$\Psi^G(\bar{x}) := \exists^{\geq k} y \left(\bigvee_{1 \leq i \leq k} \text{dist}(x_i, y) \leq 2r+1 \wedge \text{sph}_\tau(\bar{x}, y) \right).$$

Since $\text{sph}_\tau(\bar{x}, y)$ is r -local around \bar{x}, y , the formula $\Psi^G(\bar{x})$ is $(3r+1)$ -local around \bar{x} . Thus, $\Psi^G(\bar{x})$ is a formula in Gaifman normal form that is equivalent to $\Psi(\bar{x})$.

Furthermore, the size of $\Psi^G(\bar{x})$ is $O(k^2 + k \log(r) + |\text{sph}_\tau(\bar{x}, y)|) \subseteq \text{poly}(k + n\nu(r))$, and $\Psi^G(\bar{x})$ can be computed in time $\text{poly}(k + n\nu(r))$.

In Case 2 we know that y has to be far away from each of the x_i . More precisely, τ is the isomorphism type of an r -sphere around \bar{x}, y , and y has distance $> 2r+1$ from each of the x_i . Thus, we know that τ is the disjoint union of an r -sphere τ_y with center y and an r -sphere $\tau_{\bar{x}}$ with center \bar{x} . Moreover, τ_y and $\tau_{\bar{x}}$ can be computed in time $\text{poly}(|\text{sph}_\tau(\bar{x}, y)|)$.

The formula $\Psi(\bar{x})$ obviously is equivalent to the formula

$$\begin{aligned}\text{sph}_{\tau_{\bar{x}}}(\bar{x}) \wedge \exists^{\geq k} y \left(\text{sph}_{\tau_y}(y) \wedge \bigwedge_{1 \leq i \leq n} \text{dist}(x_i, y) > 2r+1 \right) \\ = \underbrace{\psi_1(\bar{x})}_{= \psi_1(\bar{x})} \wedge \underbrace{\exists^{\geq k} y \left(\text{sph}_{\tau_y}(y) \wedge \bigwedge_{1 \leq i \leq n} \text{dist}(x_i, y) > 2r+1 \right)}_{= \psi_2(\bar{x}, y)}\end{aligned}$$

While the formula $\psi_1(\bar{x})$ is in Gaifman normal form, the formula $\psi_2(\bar{x}, y)$ unfortunately is not.

Note, however, that if we know that $N_{2r+1}(\bar{x})$ contains exactly ℓ elements y that satisfy $\text{sph}_{\tau_y}(y)$, then $\psi_2(\bar{x}, y)$ is equivalent to the formula $\exists^{\geq k+\ell} y \text{sph}_{\tau_y}(y)$.

Furthermore, since we restrict attention to ν -bounded structures, we know that $N_{2r+1}(\bar{x})$ contains at most $n\nu(2r+1)$ elements, and thus it suffices to consider numbers ℓ with $0 \leq \ell \leq n\nu(2r+1)$.

Thus, $\psi_2(\bar{x}, y)$ is ν -equivalent to the formula

$$\psi_2'(\bar{x}, y) := \bigvee_{0 \leq \ell \leq n\nu(2r+1)} \left(\exists^{\geq k+\ell} y \text{sph}_{\tau_y}(y) \wedge \lambda^{\overline{\ell}}(\bar{x}) \right),$$

where for each $\ell \in \{0, \dots, n\nu(2r+1)\}$ we let

$$\begin{aligned}\lambda^{\geq \ell}(\bar{x}) &:= \exists^{\geq \ell} y \left(\bigvee_{1 \leq i \leq n} \text{dist}(x_i, y) \leq 2r+1 \wedge \text{sph}_{\tau_y}(y) \right), \\ \lambda^{\overline{\ell}}(\bar{x}) &:= \lambda^{\geq \ell}(\bar{x}) \wedge \neg \lambda^{\geq \ell+1}(\bar{x}).\end{aligned}$$

Note that the formula $\lambda^{=\ell}(\bar{x})$ is $(3r+1)$ -local around \bar{x} and thus in Gaifman normal form. It can be constructed in time $O(\ell^2 + n \log(r) + \|\text{sph}_{\tau_y}(y)\|) \subseteq \text{poly}(n\nu(2r+1))$.

Furthermore, the formula

$$\exists^{\geq k+\ell} y \text{ sph}_{\tau_y}(y)$$

is a Hanf-sentence. According to Remark III.5 it can be transformed in time $2^{O((k+\ell) \log(k+\ell))} \cdot \text{poly}(\nu(r)) \subseteq 2^{\text{poly}(k+n\nu(2r+1))}$ into an equivalent sentence $\gamma_{k+\ell}$ in Gaifman normal form.

In summary, we obtain that the given formula $\Psi(\bar{x})$ is ν -equivalent to the following formula $\Psi^G(\bar{x})$ in Gaifman normal form:

$$\Psi^G(\bar{x}) := \text{sph}_{\tau_{\bar{x}}}(\bar{x}) \wedge \bigvee_{0 \leq \ell \leq n\nu(2r+1)} \left(\gamma_{k+\ell} \wedge \lambda^{=\ell}(\bar{x}) \right).$$

Furthermore, this formula can be constructed in time

$$\text{poly}(n\nu(2r+1)) \cdot 2^{\text{poly}(k+n\nu(2r+1))} \subseteq 2^{\text{poly}(k+n\nu(2r+1))}.$$

This completes the proof of Theorem III.6. \blacksquare

C. The Gaifman normal form algorithm

We are now ready for proving Theorem III.1. When given an input $\text{FO}(\sigma)$ -formula Ψ of quantifier rank q and with free variables $\bar{x} = (x_1, \dots, x_n)$ (for $n \geq 0$), our algorithm proceeds as follows:

(1) Use Theorem II.1 to transform Ψ into a ν -equivalent formula Ψ^H in Hanf normal form.

This takes time $2^{\text{poly}(\|\Psi\| \cdot \nu(4^q))}$. The Hanf-formulas occurring in this formula are of the form $\exists^{\geq k} y \text{ sph}_{\tau}(\bar{x}, y)$, where $k \leq \|\Psi\| \cdot (q+1) \cdot \nu(4^q)$, and τ is a ν -bounded r -sphere of radius $r \leq 4^q$ with at most $n+1$ centers.

(2) Use Remark III.5 and Theorem III.6 to transform each of the Hanf-formulas occurring in Ψ^H into ν -equivalent formulas in Gaifman normal form.

For each Hanf-formula this takes time

$$2^{\text{poly}(k+n\nu(2 \cdot 4^q+1))} \subseteq 2^{\text{poly}(\|\Psi\| \cdot \nu(2 \cdot 4^q+1))}.$$

In summary, our algorithm takes time

$$2^{\text{poly}(\|\Psi\| \cdot \nu(4^q))} \cdot 2^{\text{poly}(\|\Psi\| \cdot \nu(2 \cdot 4^q+1))} \subseteq 2^{\text{poly}(\|\Psi\| \cdot \nu(2 \cdot 4^q+1))}.$$

This completes the proof of Theorem III.1. \blacksquare

IV. THE LOWER BOUND

In this section we show that the upper bound for Gaifman normal forms on classes of structures of bounded degree obtained in Theorem III.1 is basically optimal. This section's main result exposes two sequences $(\Psi_h)_{h \geq 1}$ and $(\Phi_h)_{h \geq 1}$ of FO-sentences of increasing length such that sentences in Gaifman normal form which are

- (A) ν_3 -equivalent to Ψ_h have length $2^{2^{\Omega(\|\Psi_h\|)}}$.
- (B) ν_2 -equivalent to Φ_h have length $2^{2^{\Omega(\|\Phi_h\|)}}$.

The overall structure of the proof is similar to the proof of the non-elementary lower bound of [5] on the size of Gaifman

normal forms on the class of finite forests of unbounded degree (Theorem 4.2 in [5]) — in the present paper, however, modified by a trick that saves us from having to define the arithmetic operations employed in [5] and that can also be used to improve Theorem 4.2 of [5] to obtain formulas φ_h of size $O(h)$ rather than $O(h^4)$.

The key idea is to encode large numbers by suitable structures (of degree 3 for (A) and of degree 2 for (B)) on which these numbers can be compared by small FO-formulas. For (B) we will use the encoding of [11, Section 7]. For (A) we will translate the encoding of [9, Chapter 10] into a suitable encoding by binary trees.

A. 3-fold exponential lower bound for structures of degree 3

In this subsection we consider the signature $\sigma = \{E\}$ which consists of a single binary relation symbol E . By \mathfrak{BT} we denote the class of all finite directed binary trees, i.e., finite trees where every node has at most 2 children. \mathfrak{BF} denotes the class of all finite directed binary forests, i.e., disjoint unions of finitely many elements in \mathfrak{BT} . Note that all structures in \mathfrak{BF} have degree ≤ 3 .

This subsection's main result reads as follows:

Theorem IV.1. *There is an $\varepsilon > 0$ and a sequence of $\text{FO}(E)$ -sentences $(\Psi_h)_{h \geq 1}$ of increasing size such that, for every $h \geq 1$, every sentence in Gaifman normal form that is equivalent to Ψ_h on \mathfrak{BF} has size at least $2^{2^{\varepsilon \cdot \|\Psi_h\|}}$.*

For the proof we consider the (non-elementary) function $\text{Tower}: \mathbb{N} \rightarrow \mathbb{N}$ defined by $\text{Tower}(0) := 1$ and

$$\text{Tower}(h) := 2^{\text{Tower}(h-1)} \quad \text{for all } h \geq 1.$$

We present an encoding of numbers by binary trees which enables us to define, for every $h \geq 1$, an $\text{FO}(E)$ -sentence of size $O(\text{Tower}(h))$ which can distinguish suitable pairs of forests that cannot be distinguished by any sentence in Gaifman normal form of size less than $\text{Tower}(h+3)$.

The encoding of numbers by binary trees is an adaptation of the encoding of numbers by trees of unbounded degree introduced in [9, Section 10.3]. The basic idea is to take the tree-encoding of [9] and turn it into a binary tree by replacing every node v that has $\ell > 2$ children by a complete binary tree that has $\geq \ell$ leaves. For giving a precise definition of our encoding, the following notation is convenient:

For every node a of a binary tree \mathcal{B} , we write \mathcal{B}_a for the subtree of \mathcal{B} containing all nodes that are reachable by a path starting in a . The *height* of a node a in a binary tree \mathcal{B} is the length of the path from the root of \mathcal{B} to a . The height of \mathcal{B} is the maximal height of a node in \mathcal{B} . For a binary tree \mathcal{B} and an $n \in \mathbb{N}$ we write $\mathcal{B}[\leq n]$ for the induced subtree of \mathcal{B} containing all nodes of \mathcal{B} of height $\leq n$.

\mathcal{B} is a *complete* binary tree if all leaves of \mathcal{B} have the same height and every inner node has exactly two children. By \mathcal{C}_n we denote the complete binary tree of height n .

Let $f: \mathbb{Z} \rightarrow \mathbb{N}$ be the function defined by $f(h) := 0$ ($= \text{Tower}(0) - 1$) for all $h \leq -1$ and

$$f(h) := \text{Tower}(h+1) - 1 \quad \text{for all } h \geq 0.$$

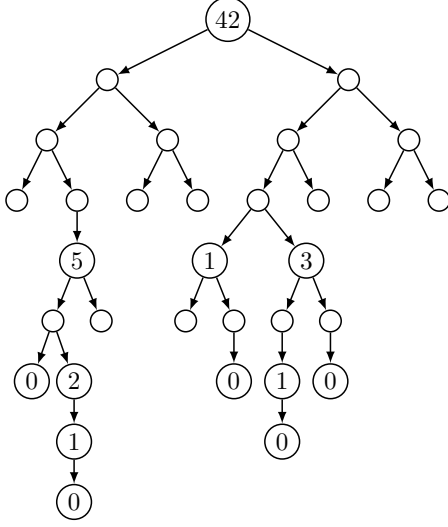


Fig. 2. An element of $\mathfrak{B}_1(42)$, i.e., a binary tree encoding of the number 42 with parameter 1. The numbers depicted within some of the nodes are *not* part of the tree encoding, they are just indicated here to illustrate which number is encoded by the subtree starting at the respective node.

Note, that for every $h \leq -1$, $\mathcal{C}_{f(h)}$ and $\mathcal{B}[\leq f(h)]$, for every binary tree \mathcal{B} , are binary trees with just one node.

For natural numbers j, i let $\text{Bit}(j, i) = \lfloor i/2^j \rfloor \bmod 2$ denote the j -th bit in the binary expansion of i . We now define, for $h' \in \mathbb{N}$ and $0 \leq i < \text{Tower}(h')$, a set $\mathfrak{B}_{h'-3}(i)$ of binary trees that (each) encode the (binary expansion of the) number i .

Definition IV.2 (Binary tree encoding). Let $h \geq -3$ and $0 \leq i < \text{Tower}(h+3)$. Then $\mathfrak{B}_h(i)$ is the set of binary trees \mathcal{B} that satisfy

- (1) $\mathcal{B}[\leq f(h)] \cong \mathcal{C}_{f(h)}$ and
- (2) For all $i' < \text{Tower}(h+2)$, $\text{Bit}(i', i) = 1$ iff there exists a node b of \mathcal{B} of height $f(h) + 1$ such that the binary tree \mathcal{B}_b is an element of $\mathfrak{B}_{h-1}(i')$.

Each tree in $\mathfrak{B}_h(i)$ is called a *binary tree encoding of i with parameter h* (see Figure 2 for an illustration).

By induction on h , one sees that every number $0 \leq i < \text{Tower}(h+3)$ has at least one binary tree encoding with parameter h : For the induction base let $h \leq -1$ and $0 \leq i \leq 3$. The number 0 is encoded by the singleton tree, the number 1 is encoded by a tree with a single edge, the number 2 by a path of length 2, and 3 by a tree with a branch of length 1 and one of length 2. (Note that in this case our binary tree encoding coincides with the tree encoding used in [5], [9].) For the induction step let $h \geq 0$. The initial complete binary tree of height $f(h)$ has $\text{Tower}(h+2)/2$ many leaves. This allows us to connect $\text{Tower}(h+2)$ many binary tree encodings with parameter $h-1$. Hence we can encode all numbers up to $\text{Tower}(h+3)-1$.

Let $h \geq -3$, $i < \text{Tower}(h+3)$ and $\mathcal{B} \in \mathfrak{B}_h(i)$. We say that a subtree \mathcal{B}' of \mathcal{B} encodes bit i' of i if $\mathcal{B}' \in \mathfrak{B}_{h-1}(i')$ and the

height of the root of \mathcal{B}' in \mathcal{B} is $f(h) + 1 = \text{Tower}(h+1)$.

Lemma IV.3. *There is a sequence of FO(E)-formulas $(\text{eq}_h(x, y))_{h \geq -3}$ of size $\|\text{eq}_h\| \in O(\text{Tower}(h))$ (for $h \geq 0$) such that for every binary forest \mathcal{B} and all nodes a, b of \mathcal{B} the following holds: If $\mathcal{B}_a \in \mathfrak{B}_h(i)$ and $\mathcal{B}_b \in \mathfrak{B}_h(j)$, for numbers $i, j < \text{Tower}(h+3)$, then $\mathcal{B} \models \text{eq}_h[a, b]$ iff $i = j$.*

Proof: For the proof it will be convenient to use the fact that for every $r \in \mathbb{N}$ there is an FO(E)-formula $\delta_r(x, y)$ of size $O(\log(r))$ expressing in a directed graph G that there is a directed path of length exactly r from node x to node y . The formulas $\delta_0(x, y)$ and $\delta_1(x, y)$ can be chosen as $x=y$ and $E(x, y)$, respectively, and for every $r \geq 1$ we can choose

$$\delta_{2r}(x, y) := \exists u \forall v \forall w ((v=x \wedge w=u) \vee (v=u \wedge w=y)) \rightarrow \delta_r(v, w),$$

$$\delta_{2r+1}(x, y) := \exists z (E(x, z) \wedge \delta_{2r}(z, y)).$$

Let us now turn to the proof of Lemma IV.3. For $h \in \{-3, -2, -1\}$, the formulas $\text{eq}_h(x, y)$ can be chosen in a straightforward way. In the following we describe the construction of the formulas $\text{eq}_h(x, y)$ for $h \geq 0$.

Let \mathcal{B} be a binary forest, and let a and b be nodes of \mathcal{B} such that \mathcal{B}_a and \mathcal{B}_b are binary tree encodings in $\mathfrak{B}_h(i)$ and $\mathfrak{B}_h(j)$, respectively, for numbers $i, j < \text{Tower}(h+3)$. The formula $\text{eq}_h(x, y)$ shall be satisfied by a, b , iff for every root node a' of a subtree of \mathcal{B}_a encoding a bit of i there is a root node b' of a subtree of \mathcal{B}_b encoding a bit of j such that $\mathcal{B} \models \text{eq}_{h-1}[a', b']$, and vice versa. Note that a' is a root node of a subtree of \mathcal{B}_a encoding a bit of i if, and only if, there is a directed path of length exactly $\text{Tower}(h+1)$ from a to a' .

Therefore, the formulas $\text{eq}_h(x, y)$ can be chosen in the same way as the according formulas in [9, Lemma 10.21]; the only modification we need to do is to replace atoms of the form $E(u, v)$ by the formula $\delta_{\text{Tower}(h+1)}(u, v)$, expressing that there is a directed path of length exactly $\text{Tower}(h+1)$ from u to v . This leads, for every $h \geq 0$, to the formula $\text{eq}_h(x, y) :=$

$$\begin{aligned} & \left(\exists x' \delta_{\text{Tower}(h+1)}(x, x') \leftrightarrow \exists y' \delta_{\text{Tower}(h+1)}(y, y') \right) \wedge \\ & \forall x' \left(\delta_{\text{Tower}(h+1)}(x, x') \rightarrow \exists y' \left(\delta_{\text{Tower}(h+1)}(y, y') \wedge \right. \right. \\ & \quad \left. \left. \forall y'' \left(\delta_{\text{Tower}(h+1)}(y, y'') \rightarrow \exists x'' \left(\delta_{\text{Tower}(h+1)}(x, x'') \wedge \right. \right. \right. \right. \\ & \quad \left. \left. \left. \forall u \forall v \left(((u = x' \wedge v = y') \vee (u = x'' \wedge v = y'')) \right. \right. \right. \right. \\ & \quad \left. \left. \left. \rightarrow \text{eq}_{h-1}(u, v) \right) \right) \right) \right) \end{aligned}$$

Note that the formula $\delta_{\text{Tower}(h+1)}$ has length $O(\log(\text{Tower}(h+1))) = O(\text{Tower}(h))$, and thus the formula eq_h has size $\|\text{eq}_h\| = O(\text{Tower}(h)) + \|\text{eq}_{h-1}\|$. Inductively, this leads to $\|\text{eq}_h\| \in O(\sum_{i=0}^h \text{Tower}(i))$. An easy induction shows, that $\sum_{i=0}^h \text{Tower}(i) < 2 \cdot \text{Tower}(h)$ for all $h \geq 0$. Hence, $\|\text{eq}_h\| \in O(\text{Tower}(h))$. ■

We are now ready for the proof of Theorem IV.1.

Proof of Theorem IV.1: Let $h \geq 1$. Let us fix, for every $i < \text{Tower}(h+3)$, a binary tree encoding $\mathcal{B}_{h,i}$ of i with parameter h , i.e., $\mathcal{B}_{h,i} \in \mathfrak{B}_h(i)$.

We let $H := \text{Tower}(h+3)$ and we let \mathcal{A}_h be the structure consisting of *two* disjoint copies of every structure $\mathcal{B}_{h,i}$ for all $i \in \{0, \dots, H-1\}$. For every $j < H$ we let \mathcal{A}_h^{-j} be the structure obtained from \mathcal{A}_h by removing *one* copy of $\mathcal{B}_{h,j}$.

Note that \mathcal{A}_h and \mathcal{A}_h^{-j} are binary forests. The roots of the trees in these forests are exactly the nodes x satisfying $\text{root}(x) := \neg \exists y E(y, x)$. The formula Ψ_h is now chosen as follows:

$$\forall x (\text{root}(x) \rightarrow \exists y (\text{root}(y) \wedge \text{eq}_h(x, y) \wedge \neg x=y)),$$

where $\text{eq}_h(x, y)$ is the formula of length $O(\text{Tower}(h))$ obtained from Lemma IV.3. Thus, $\|\Psi_h\| = O(\text{Tower}(h))$.

Note that, when evaluated in \mathcal{A}_h or \mathcal{A}_h^{-j} , the formula Ψ_h states that for every tree $\mathcal{B}_{h,i}$ present in the structure, there is a second copy of $\mathcal{B}_{h,i}$. Thus

$$\mathcal{A}_h \models \Psi_h \text{ and } \mathcal{A}_h^{-j} \not\models \Psi_h, \text{ for all } j < H. \quad (3)$$

Now assume Φ is a formula in Gaifman normal form that is equivalent to Ψ_h on the class \mathfrak{BF} of all finite binary forests. In particular, since \mathcal{A}_h as well as each of the structures \mathcal{A}_h^{-j} belong to \mathfrak{BF} , we obtain from (3) that

$$\mathcal{A}_h \models \Phi \text{ and } \mathcal{A}_h^{-j} \not\models \Phi, \text{ for all } j < H. \quad (4)$$

To complete the proof, it suffices to show that $\|\Phi\| \geq H$ (recall that $H = \text{Tower}(h+3) = 2^{2^{\text{Tower}(h)}}$ and $\|\Psi_h\| = O(\text{Tower}(h))$). For contradiction, assume that $\|\Phi\| < H$.

From here on, the proof is virtually identical to the proof of Theorem 4.2 in [5]: Since Φ is in Gaifman normal form, it is a Boolean combination of basic local sentences χ_1, \dots, χ_L , for an $L \geq 1$, where each χ_ℓ (for $1 \leq \ell \leq L$) is of the form

$$\exists x_1 \dots \exists x_{k_\ell} \left(\bigwedge_{1 \leq i < j \leq k_\ell} \text{dist}(x_i, x_j) > 2r_\ell \wedge \bigwedge_{1 \leq i \leq k_\ell} \psi_\ell(x_i) \right)$$

for numbers $k_\ell, r_\ell \geq 1$ and r_ℓ -local formulas $\psi_\ell(x)$.

In particular, $\|\Phi\| \geq k_1 + \dots + k_L$. We can assume w.l.o.g. that there exists an \tilde{L} with $0 \leq \tilde{L} \leq L$ such that

$$\mathcal{A}_h \models \chi_\ell \text{ for all } \ell \leq \tilde{L}, \text{ and } \mathcal{A}_h \not\models \chi_\ell \text{ for all } \ell > \tilde{L}. \quad (5)$$

For each $\ell \leq \tilde{L}$ we know that $\mathcal{A}_h \models \chi_\ell$, i.e., there are nodes $t_1^{(\ell)}, \dots, t_{k_\ell}^{(\ell)}$ in \mathcal{A}_h such that the formula

$$\bigwedge_{1 \leq i < j \leq k_\ell} \text{dist}(x_i, x_j) > 2r_\ell \wedge \bigwedge_{1 \leq i \leq k_\ell} \psi_\ell(x_i) \quad (6)$$

is satisfied in \mathcal{A}_h when interpreting the variables x_i with the nodes $t_i^{(\ell)}$. The set $T := \{t_i^{(\ell)} : 1 \leq \ell \leq \tilde{L} \text{ and } 1 \leq i \leq k_\ell\}$ consists of at most $k_1 + \dots + k_{\tilde{L}} \leq \|\Phi\|$ nodes, which, by assumption, is $< H$.

Note that \mathcal{A}_h consists of $2H$ trees. Since $|T| < H$, one of the trees \mathcal{B} of \mathcal{A}_h does not contain any element of T , and there is a $j \in \{0, \dots, H-1\}$ such that $\mathcal{B} \cong \mathcal{B}_{h,j}$.

Thus, the structure \mathcal{A}_h^{-j} obtained from \mathcal{A}_h by removing one copy of $\mathcal{B}_{h,j}$ still contains all the nodes in T .

Considering (6), note that each formula $\psi_\ell(x_i)$ is r_ℓ -local around x_i . Thus, when interpreting x_i with the node $t_i^{(\ell)}$, the formula can only speak about the r_ℓ -neighborhood of $t_i^{(\ell)}$ —

and this is the same in \mathcal{A}_h^{-j} as in \mathcal{A}_h . We thus obtain from (6) that $\mathcal{A}_h^{-j} \models \chi_\ell$ for each $\ell \leq \tilde{L}$.

Let us now consider the formulas χ_ℓ with $\ell > \tilde{L}$. From (5) we know that $\mathcal{A}_h \not\models \chi_\ell$. However, assuming that $\mathcal{A}_h^{-j} \models \chi_\ell$ and noting that \mathcal{A}_h is the disjoint union of \mathcal{A}_h^{-j} with another structure, the fact that χ_ℓ is a basic local sentence immediately leads to the (contradicting) conclusion that also $\mathcal{A}_h \models \chi_\ell$.

In summary, we now know the following:

$$\mathcal{A}_h^{-j} \models \chi_\ell \text{ for all } \ell \leq \tilde{L}, \text{ and } \mathcal{A}_h^{-j} \not\models \chi_\ell \text{ for all } \ell > \tilde{L}. \quad (7)$$

From (7) and (5) we know that \mathcal{A}_h^{-j} satisfies the same basic local sentences from $\{\chi_1, \dots, \chi_L\}$ as \mathcal{A}_h . Since Φ is a Boolean combination of these sentences, we obtain that

$$\mathcal{A}_h^{-j} \models \Phi \iff \mathcal{A}_h \models \Phi.$$

This, however, is a contradiction to (4). Altogether, the proof of Theorem IV.1 is complete. ■

With the analogous proof, one also obtains the following strengthening of Theorems 4.1 and 4.2 of [5] with formulas φ_h of size $O(h)$ rather than $O(h^4)$:

Corollary IV.4. *For every $h \geq 1$ there is an FO(E)-sentence φ_h of size $O(h)$ such that every FO(E)-sentence in Gaifman normal form that is equivalent to φ_h on the class $\mathfrak{F}_{\leq h}$ of finite forests of height $\leq h$ has size at least $\text{Tower}(h)$.*

The same holds true when replacing the class $\mathfrak{F}_{\leq h}$ with the class \mathfrak{T} of all finite trees.

Proof: It suffices to modify the first two paragraphs of [5]’s proof of Theorem 4.2 as follows: [5] defines \mathcal{F}_h to be the forest that consists of the disjoint union of all trees $\mathcal{T}(j)$ (defined in [5]), for all $j \in \{0, \dots, \text{Tower}(h)-1\}$. Instead, we now let \mathcal{F}_h consist of *two* disjoint copies of $\mathcal{T}(j)$, for all j with $0 \leq j < \text{Tower}(h)$. For every $i < \text{Tower}(h)$, we let \mathcal{F}_h^{-i} be the forest obtained from \mathcal{F}_h by removing *one* copy of $\mathcal{T}(i)$. Now, φ_h is chosen as

$$\forall x (\text{root}(x) \rightarrow \exists y (\text{root}(y) \wedge \text{eq}_h(x, y) \wedge \neg x=y)),$$

where $\text{root}(x) := \neg \exists y E(y, x)$, and where $\text{eq}_h(x, y)$ is the formula of length $O(h)$ obtained from [9, Lemma 10.21].

Clearly, φ_h is of length $O(h)$, and

$$\mathcal{F}_h \models \varphi_h \text{ and } \mathcal{F}_h^{-i} \not\models \varphi_h, \text{ for all } i < \text{Tower}(h).$$

The rest of the proof can be taken verbatim from the proof of Theorem 4.2 of [5]. ■

Remark IV.5. In the same way as the result of [5] holds for trees as well as for forests, our Theorem IV.1 can be generalised to the class \mathfrak{BT} of all finite binary trees. We sketch the basic idea of the proof here; for details see the full version of this paper. To obtain the tree $\mathcal{A}_{h,R}$, we start with a “very long” branch a_0, a_1, \dots, a_m where m depends on R and on h . At “very long distances” (depending on R), we attach two copies of each of the trees $\mathcal{B}_{h,i}$ to this branch. The tree $\mathcal{A}_{h,R}^{-j}$ is obtained from $\mathcal{A}_{h,R}$ by deleting one copy of $\mathcal{B}_{h,j}$. Since the paths between the trees $\mathcal{B}_{h,i}$ are extremely

long, they cannot be bridged by “small” formulas in Gaifman normal form and therefore act as if they were not present. This allows to treat $\mathcal{A}_{h,R}$ and $\mathcal{A}_{h,R}^{-j}$ similarly to \mathcal{A}_h and \mathcal{A}_h^{-j} in the above proof of Theorem IV.1.

B. 2-fold exponential lower bound for structures of degree 2

We now consider the signature $\sigma = \{S, P_0, P_1\}$ consisting of a binary relation symbol S and two unary relation symbols. A *labeled chain* is a finite σ -structure \mathcal{C} whose S -reduct is a chain of finite length, i.e., a finite directed path, and where the sets $P_0^{\mathcal{C}}$ and $P_1^{\mathcal{C}}$ are disjoint subsets of the universe of \mathcal{C} . We write \mathfrak{LC} to denote the class of all σ -structures that are disjoint unions of finitely many labeled chains. Note that all structures in \mathfrak{LC} have degree ≤ 2 .

This subsection’s main result reads as follows:

Theorem IV.6. *There is an $\varepsilon > 0$ and a sequence of FO(σ)-sentences $(\Psi_h)_{h \geq 1}$ of increasing size such that, for every $h \geq 1$, every sentence in Gaifman normal form that is equivalent to Ψ_h on \mathfrak{LC} has size at least $2^{2^{\varepsilon \cdot \|\Psi_h\|}}$.*

The proof has the same overall structure as the proof of Theorem IV.1. Now, however, instead of using the binary tree encodings from Definition IV.2, we employ the obvious encodings of numbers by strings: Let $\Sigma = \{0, 1\}$. For $h \geq 1$ and $i < 2^{2^h}$ let $\text{bin}_{2^h}(i)$ denote the binary expansion of i of length 2^h .

Strings $w \in \Sigma^+$ are represented as σ -structures \mathcal{B}_w in the usual way: the universe of \mathcal{B}_w is the set of positions of the string w , the relation $S^{\mathcal{B}_w}$ is the successor relation on the positions of w , and $P_a^{\mathcal{B}_w}$ consists, for each $a \in \Sigma$, of all positions of w that carry the letter a .

For the proof of Theorem IV.6 we will use structures \mathcal{B}_w for strings $w = \text{bin}_{2^h}(i)$ with $i \in \{0, \dots, 2^{2^h} - 1\}$, and we will rely on the following result of [11].

Lemma IV.7 (Lemma 20 in [11]). *There is a sequence of FO(σ)-formulas $(\tilde{\text{eq}}_h(x, y))_{h \geq 1}$ of size $\|\tilde{\text{eq}}_h(x, y)\| \in O(h)$ such that for all structures $\mathcal{B} \in \mathfrak{LC}$ and all nodes a, b of \mathcal{B} the following holds: If a and b are the starting positions of labeled chains isomorphic to $\mathcal{B}_{\text{bin}_{2^h}(i)}$ and $\mathcal{B}_{\text{bin}_{2^h}(j)}$, respectively, for $i, j \in \{0, \dots, 2^{2^h} - 1\}$, then $\mathcal{B} \models \tilde{\text{eq}}_h[a, b]$ iff $i = j$.*

Proof of Theorem IV.6: Let $h \geq 1$, $H := 2^{2^h}$, and $\mathcal{B}_{h,i} = \mathcal{B}_{\text{bin}_{2^h}(i)}$ for all $i < H$. We let $\mathcal{A}_h \in \mathfrak{LC}$ be the structure consisting of the disjoint union of two copies of the labeled chains $\mathcal{B}_{h,i}$ for all $i \in \{0, \dots, H-1\}$.

For every $j \in \{0, \dots, H-1\}$ we let \mathcal{A}_h^{-j} be the structure obtained from \mathcal{A}_h by removing one copy of $\mathcal{B}_{h,j}$.

Note that the starting points of disjoint copies of labeled chains in \mathcal{A}_h are exactly the nodes x satisfying the formula $\text{root}(x) := \neg \exists y S(y, x)$. The formula Ψ_h is now chosen as

$$\forall x (\text{root}(x) \rightarrow \exists y (\text{root}(y) \wedge \tilde{\text{eq}}_h(x, y) \wedge \neg x=y)),$$

where $\tilde{\text{eq}}_h(x, y)$ is the formula of length $O(h)$ obtained from Lemma IV.7. Thus, $\|\Psi_h\| = O(h)$.

Note that, when evaluated in \mathcal{A}_h or in one of the structures \mathcal{A}_h^{-j} , the formula Ψ_h states that for every copy of $\mathcal{B}_{h,i}$

present in the structure, there is a second copy of $\mathcal{B}_{h,i}$. Thus, obviously, the following is true:

$$\mathcal{A}_h \models \Psi_h \quad \text{and} \quad \mathcal{A}_h^{-j} \not\models \Psi_h, \quad \text{for all } j < H.$$

The rest of the proof can be taken almost verbatim from the proof of Theorem IV.1. \blacksquare

Remark IV.8. Analogously to Remark IV.5, Theorem IV.6 even holds when replacing the class \mathfrak{LC} of disjoint unions of labeled chains with the class \mathfrak{C} of labeled chains. The basic idea is to put all the chains of \mathcal{A}_h and \mathcal{A}_h^{-j} into one single chain, interspersed by long sequences of nodes not belonging to any of P_0 or P_1 . Details can be found in the full version of this paper.

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