An Existential Locality Theorem

Martin Grohe[1] and Stefan Wöhrle[2]

[1] Laboratory for Foundations of Computer Science, University of Edinburgh, Edinburgh EH9 3JZ, Scotland, UK.
grohe@dcs.ed.ac.uk
[2] Lehrstuhl für Informatik VII, RWTH Aachen, 52056 Aachen, Germany.
woehrle@informatik.rwth-aachen.de

Abstract. We prove an existential version of Gaifman's locality theorem and show how it can be applied algorithmically to evaluate existential first-order sentences in finite structures.

1 Introduction

Gaifman's locality theorem [12] states that every first-order sentence is equivalent to a Boolean combination of sentences saying: There exist elements $a_1, \ldots, a_k$ that are far apart from one another, and each a_i satisfies some local condition described by a first-order formula whose quantifiers only range over a fixed-size neighborhood of an element of a structure. We prove that every *existential* first-order sentence is equivalent to a *positive* Boolean combination of sentences saying: There exist elements $a_1, \ldots, a_k$ that are far apart from one another, and each a_i satisfies some local condition described by an *existential* first-order formula.

The locality of first-order logic can be explored to prove that certain properties of finite structures are not expressible in first-order logic, and it seems that this was Gaifman's main motivation. More recently, Libkin and others considered this technique of proving inexpressibility results using locality in a complexity theoretic context (see, e.g., [5, 15, 14, 16]).

A completely different application of Gaifman's theorem has been proposed in [11]: It can be used to evaluate first-order sentences in certain finite structures quite efficiently. In general, it takes time $n^{\Theta(l)}$ to decide whether a structure of size n satisfies a first-order sentence of size l, and under complexity theoretic assumptions, it can be proved that no real improvement is possible: The problem of deciding whether a given structure satisfies a given first-order sentence is PSPACE-complete [18, 20], and if parameterized by the size of the input sentence, it is complete for the parameterized complexity class AW[$*$] [7]. The latter result implies that it is unlikely that the problem is fixed-parameter tractable (cf. [6]), i.e., that it can be solved in time $f(l) \cdot n^c$, for a function f and a constant c.

Gaifman's theorem reduces the question of whether a first-order sentence holds in a structure to the question of whether the structure contains elements that are far apart from one another and satisfy some local condition expressed by a first-order formula. In certain structures, it is much easier to decide whether an element satisfies a local first-order formula than to decide whether the whole structure satisfies a first-order sentence. An example are graphs of bounded degree: Local neighborhoods of vertices in such graphs have a size bounded by a constant only depending on the radius of the neighborhoods, so the time needed to check whether a vertex satisfies a local condition does not depend on the size of the graph. Another, less obvious example are planar graphs. To evaluate local conditions in planar graphs, we can exploit the fact that in planar graphs neighborhoods of fixed radius have bounded tree-width [17]. In general, such a locality based approach to evaluating first-order sentences in finite structures works for classes of structures that have a property called bounded local tree-width; the class of planar graphs and all classes of structures of bounded degree are examples of classes having this property. It has been proved in [11] that for each class C of structures of bounded local tree-width there is an algorithm that, given a structure $\mathcal{A} \in$ C and a first-order sentence φ, decides whether $\mathcal{A}$ satisfies φ in time near linear in the size of the structure $\mathcal{A}$ (the precise statement is Theorem 7).

While a linear dependence on the size of the input structure is optimal, the dependence of these algorithms on the size of the input sentence leaves a lot to be desired: There is not even an elementary upper bound for the runtime in terms of the size of the sentence. Although the dependence of the algorithm on the structure size matters much more than the dependence on the size of the sentence, because usually we are evaluating small sentences in large structures,[1] it would be desirable to have a dependence on the size of the sentence that is not worse than exponential. Of course, since we are dealing with a PSPACE complete problem, we cannot expect the runtime of an algorithm to be polynomial in both the size of the input structure and the size of the input sentence.

We have observed that one of the main factors contributing to the enormous runtime of the locality based algorithms in terms of the formulas size is the number of quantifier alternations in the formula. This has motivated the present paper. We can use a variant of our existential locality theorem to improve the algorithms described above to algorithms whose runtime "only" depends doubly exponentially on the size of the input sentence.

In this paper we concentrate on the proof of our existential locality theorem, which is surprisingly complicated. This proof is presented in Section 3. The algorithmic application is outlined in Section 4.

2 Preliminaries

A *vocabulary* is a finite set of relation symbols. Associated with every relation symbol R is a positive integer called the *arity* of R. In the following, τ always denotes a vocabulary.

A τ*-structure* $\mathcal{A}$ consists of a non-empty set A, called the *universe* of $\mathcal{A}$, and a relation $R^{\mathcal{A}} \subseteq A^r$ for each r-ary relation symbol $R \in \tau$. For instance, we consider *graphs* as $\{E\}$-structures $\mathcal{G} = (G, E^{\mathcal{G}})$, where the binary relation $E^{\mathcal{G}}$ is symmetric and anti-reflexive (i.e. graphs are undirected and loop-free). If $\mathcal{A}$ is a τ-structure and

[1] The generic example is the problem of evaluating SQL database queries against finite relational databases, which can be modeled by the problem of evaluating first-order sentences in finite structures.

$B \subseteq A$, then $\langle B \rangle^{\mathcal{A}}$ denotes the substructure induced by $\mathcal{A}$ on B, that is, the τ-structure $\mathcal{B}$ with universe B and $R^{\mathcal{B}} := R^{\mathcal{A}} \cap B^r$ for every r-ary $R \in \tau$.

The formulas of *first-order logic* are build up from *atomic formulas* using the usual Boolean connectives and existential and universal quantification over the elements of the universe of a structure. Remember that an *atomic formula*, or *atom*, is a formula of the form $x = y$ or $R(x_1, \ldots, x_r)$, where R is an r-ary relation symbol. The set of all variables of a formula φ is denoted by $\mathrm{var}(\varphi)$. A *free variable* in a first-order formula is a variable x not in the scope of a quantifier $\exists x$ or $\forall x$. The set of all free variables of a formula φ is denoted by $\mathrm{free}(\varphi)$. A *sentence* is a formula without free variables. The notation $\varphi(x_1, \ldots, x_k)$ indicates that all free variables of the formula φ are among $x_1, \ldots, x_k$; it does not necessarily mean that the variables $x_1, \ldots, x_k$ all appear in φ. For a formula $\varphi(x_1, \ldots, x_k)$, a structure $\mathcal{A}$, and $a_1, \ldots, a_k \in A$ we write $\mathcal{A} \models \varphi(a_1, \ldots, a_k)$ to say that $\mathcal{A}$ satisfies φ if the variables $x_1, \ldots, x_k$ are interpreted by the vertices $a_1, \ldots, a_k$, respectively.

The *weight* of a first-order formula φ is the number of quantifiers $\exists x$ and $\forall x$ occurring in φ.

A first-order formula is *existential* if it contains no universal quantifiers and if every existential quantifier occurs in the scope of an even number of negation symbols. A *literal* is an atom or a negated atom. A *conjunctive query with negation* is a formula of the form $\exists \bar{x} \bigwedge_{i=1}^{m} \lambda_i$, where each λ_i is a literal. Every existential formula φ of weight w and length l is equivalent to a disjunction of at most 2^l conjunctive queries with negation, each of which is of weight at most w and length at most l.

We often denote tuples $a_1 \ldots a_k$ of elements of a set A by $\bar{a}$, and we write $\bar{a} \in A$ instead of $\bar{a} \in A^k$. Similarly, we denote tuples of variables by $\bar{x}$.

Our underlying model of computation is the standard RAM-model with addition and subtraction as arithmetic operations (cf. [1, 19]). In our complexity analysis we use the uniform cost measure. Structures are represented on a RAM in a straightforward way by listing all elements of the universe and then all tuples in the relations. For details we refer the reader to [10]. We define the *size* of a τ-structure $\mathcal{A}$ to be $||\mathcal{A}|| := |A| + \sum_{R \in \tau \ r\text{-ary}} r \cdot |R^{\mathcal{A}}|$; this is the length of a reasonable representation of $\mathcal{A}$ (if we suppress details that are inessential for us). We fix some reasonable encoding for first-order formulas and denote by $||\varphi||$ the size of the encoding of a formula φ.

2.1 Gaifman's Locality Theorem

The *Gaifman graph* of a τ-structure $\mathcal{A}$ is the graph $\mathcal{G}_{\mathcal{A}}$ with vertex set A and an edge between two vertices $a, b \in A$ if there exists an $R \in \tau$ and a tuple $a_1 \ldots a_k \in R^{\mathcal{A}}$ such that $a, b \in \{a_1, \ldots, a_k\}$. The *distance* $d^{\mathcal{A}}(a, b)$ between two elements $a, b \in A$ of a structure $\mathcal{A}$ is the length of the shortest path in $\mathcal{G}_{\mathcal{A}}$ connecting a and b. For $r \geq 1$ and $a \in A$, we define the *r-neighborhood* of a in $\mathcal{A}$ to be $N_r^{\mathcal{A}}(a) := \{b \in A \mid d^{\mathcal{A}}(a, b) \leq r\}$. For a subset $B \subseteq A$ we let $N_r^{\mathcal{A}}(B) := \bigcup_{b \in B} N_r^{\mathcal{A}}(b)$.

For every $r \geq 0$ there is an existential first-order formula $\delta_r(x, y)$ such that for all τ-structures $\mathcal{A}$ and $a, b \in A$ we have $\mathcal{A} \models \delta_r(a, b)$ if, and only if, $d^{\mathcal{A}}(a, b) \leq r$. In the following, we write $d(x, y) \leq r$ instead of $\delta_r(x, y)$ and $d(x, y) > r$ instead of $\neg \delta_r(x, y)$.

If $\varphi(x)$ is a first-order formula, then $\varphi^{N_r(x)}(x)$ is the formula obtained from $\varphi(x)$ by relativizing all quantifiers to $N_r(x)$, that is, by replacing every subformula of the form $\exists y \psi(x, y, \bar{z})$ by $\exists y(d(x, y) \leq r \wedge \psi(x, y, \bar{z}))$ and every subformula of the form $\forall y \psi(x, y, \bar{z})$ by $\forall y(d(x, y) \leq r \rightarrow \psi(x, y, \bar{z}))$. We usually write $\exists y \in N_r(x)\ \psi$ instead of $\exists y(d(x, y) \leq r \wedge \psi)$ and $\forall y \in N_r(x)\ \psi$ instead of $\forall y(d(x, y) \leq r \rightarrow \psi)$.

A formula $\psi(x)$ of the form $\varphi^{N_r(x)}(x)$, for some $\varphi(x)$, is called r-*local*. The basic property of r-local formulas $\psi(x)$ is that it only depends on the r-neighborhood of x whether they hold at x or not, that is, for all structures $\mathcal{A}$ and $a \in A$ we have $\mathcal{A} \models \psi(a)$ if, and only if, $\langle N_r^{\mathcal{A}}(a) \rangle \models \psi(a)$. Observe that if $\psi(x)$ is r-local and $s > r$, then $\psi(x)$ is equivalent to the s-local formula $\psi^{N_s(x)}(x)$. We often use this observation implicitly when considering r-local formulas as s-local for some $s > r$.

Sentences can never be local in the sense just defined. As a substitute, we say that a *local sentence* is a sentence of the form

$$\exists x_1 \ldots \exists x_k \Big(\bigwedge_{1 \leq i < j \leq k} d(x_i, x_j) > 2r \wedge \bigwedge_{1 \leq i \leq k} \psi(x_i) \Big),$$

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

Theorem 1 (Gaifman [12]). *Every first-order sentence is equivalent to a Boolean combination of local sentences.*

3 The Existential Locality Theorems

If $\psi(x)$ is an existential first-order formula, then for every $r \geq 1$ the r-local formula $\psi^{N_r(x)}(x)$ obtained from ψ is also existential. We define a local sentence

$$\exists x_1 \ldots \exists x_k \Big(\bigwedge_{1 \leq i < j \leq k} d(x_i, x_j) > 2r \wedge \bigwedge_{1 \leq i \leq k} \psi(x_i) \Big)$$

to be *existential* if the formula ψ is existential and r-local. Let us remark that, in general, an existential local sentence is *not* equivalent to an existential first-order sentence, because the formula $d(x_i, x_j) > s$ is not existential for any $s \geq 2$.

Theorem 2. *Every existential first-order sentence is equivalent to a positive Boolean combination of existential local sentences.*

Unfortunately, neither Gaifman's original proof of his locality theorem (based on quantifier elimination) nor Ebbinghaus and Flum's [8] model theoretic proof can be adapted to prove this existential version of Gaifman's theorem. Compared to these proofs, our proof is very combinatorial, which is not surprising, because there is not much "logic" left in existential sentences.

We illustrate the basic idea by a simple example:

Example 3. Let

$$\varphi := \exists x \exists y \big(\neg E(x, y) \wedge \mathrm{RED}(x) \wedge \mathrm{BLUE}(y) \big)$$

(here E is a binary relation symbol and $\textsc{Red}, \textsc{Blue}$ are unary relation symbols). Although the syntactical form of φ is close to that of an existential local sentence, it is not obvious how to find a positive Boolean combination of existential local sentences equivalent to φ. Here is one:

$$\begin{aligned}&\Big(\quad \exists x \exists y \big(d(x,y) > 2 \wedge (\textsc{Red}(x) \vee \textsc{Blue}(y)) \wedge (\textsc{Red}(y) \vee \textsc{Blue}(y)) \big) \\ &\quad \wedge \exists x\ \textsc{Red}(x) \wedge \exists x\ \textsc{Blue}(x) \Big) \\ &\vee \exists x\ \exists x' \in N_2(x) \exists y \in N_2(x) \big(\neg E(x', y) \wedge \textsc{Red}(x') \wedge \textsc{Blue}(y) \big).\end{aligned}$$

To understand the following proof it is worthwhile trying to extend the idea of this example to the sentence

$$\exists x \exists y \exists z \big(\neg E(x,y) \wedge \neg E(x,z) \wedge \neg E(y,z) \wedge \textsc{Red}(x) \wedge \textsc{Blue}(y) \wedge \textsc{Green}(z) \big)$$

(although it is very complicated to actually write down an equivalent positive Boolean combination of existential local sentences). Indeed, it is the main difficulty of the proof to handle sentences saying "there is an independent set of points $x_1, \ldots, x_k$ of colors $c_1, \ldots, c_k$, respectively." Playing with such sentences leads to the crucial observation that the basic combinatorial problem can be handled by the marriage theorem (as it is done in Step 4 of the proof of Lemma 4).

The proof requires some preparation. We define the *rank* of a local sentence

$$\exists x_1 \ldots \exists x_k \Big(\bigwedge_{1 \le i < j \le k} d(x_i, x_j) > 2r \wedge \bigwedge_{1 \le i \le k} \psi(x_i) \Big),$$

to be the pair $(k + w, r)$, where w is the weight of ψ. We partially order the ranks by saying that $(q, r) \le (q', r')$ if $q \le q'$ and $r \le r'$.

Lemma 4. *Let $k \ge 2$, $r \ge 1$, $w \ge 0$, and let $\mathcal{A}$, $\mathcal{B}$ be structures such that every existential local sentence of rank at most $(k \cdot (w+1), 2^{k^2} r)$ that holds in $\mathcal{A}$ also holds in $\mathcal{B}$. Let*

$$\varphi := \exists x_1 \ldots \exists x_k \Big(\bigwedge_{1 \le i < j \le k} d(x_i, x_j) > 2^{k^2} r \wedge \bigwedge_{i=1}^{k} \psi_i(x_i) \Big),$$

where for $1 \le i \le k$, the formula $\psi_i(x_i)$ is r-local, existential and of weight at most w. Suppose that $\mathcal{A} \models \varphi$.

Then

$$\mathcal{B} \models \exists x_1 \ldots \exists x_k \Big(\bigwedge_{1 \le i < j \le k} d(x_i, x_j) > 2r \wedge \bigwedge_{i=1}^{k} \psi_i(x_i) \Big).$$

Proof: We prove the lemma in four steps.

Step 1. We show that if for some $l, 1 \le l \le k$, say $l = k$, there are $b_1, \ldots, b_k \in B$ such that $d(b_i, b_j) > 4r$ for $1 \le i < j \le k$, and $\mathcal{B} \models \psi_l(b_i)$ for $1 \le i \le k$, then it suffices to prove that

$$\mathcal{B} \models \exists x_1 \ldots \exists x_{k-1} \Big(\bigwedge_{1 \le i < j \le k-1} d(x_i, x_j) > 2r \wedge \bigwedge_{i=1}^{k-1} \psi_i(x_i) \Big).$$

To see this, suppose that we have such $b_1, \ldots, b_k$ and we find $c_1, \ldots, c_{k-1}$ such that $d(c_i, c_j) > 2r$ for all $1 \leq i < j \leq k-1$, and $\mathcal{B} \models \psi_i(c_i)$ for $1 \leq i \leq k-1$. Then there will be at least one $i, 1 \leq i \leq k$ such that b_i has distance greater than $2r$ from c_j for all $j, 1 \leq j \leq k-1$. Thus $c_1, \ldots, c_{k-1}, b_i$ witness that

$$\mathcal{B} \models \exists x_1 \ldots \exists x_k \Big(\bigwedge_{1 \leq i < j \leq k} d(x_i, x_j) > 2r \wedge \bigwedge_{i=1}^{k} \psi_i(x_i) \Big).$$

So without loss of generality, in the following we assume that for $1 \leq i \leq k$, there are at most $(k-1)$ elements of B of pairwise distance greater than $4r$ satisfying ψ_i.

Step 2. We let $K := \{1, \ldots, k\}$, and for every set $I \subseteq K$ we let $\psi_I(x) := \bigvee_{i \in I} \psi_i(x)$. Note that ψ_I is a formula of weight at most $k \cdot w$. Let $C := \{c \in B \mid \mathcal{B} \models \psi_K(c)\}$. By the assumption we made at the end of Step 1, there exist at most $k(k-1)$ elements of C of pairwise distance greater than $4r$.

Claim: There are $p, l, 1 \leq p \leq k(k-1)+1, 1 \leq l \leq k(k-1)$, and elements $c_1, \ldots, c_l \in C$ such that $d^{\mathcal{B}}(c_i, c_j) > 2^{p+1}r$ for $1 \leq i < j \leq l$, and for all $c \in C$ there exists an $i \leq l$ such that $d^{\mathcal{B}}(c, c_i) \leq 2^p r$.

Proof: We construct $c_1, \ldots, c_l$ inductively: As the inductive basis, let c_1 be an arbitrary element of C. If $c_1, \ldots, c_i$ are constructed, we choose $c_{i+1} \in C$ such that for $1 \leq j \leq i$ we have $d^{\mathcal{B}}(c_{i+1}, c_j) > 2^{k(k-1)+1-(i-1)}r$. If no such c_{i+1} exists, we let $l := i, p := k(k-1)+1-(l-1)$ and stop.

Our construction guarantees that for $1 \leq i < j \leq l$ we have

$$d^{\mathcal{B}}(c_i, c_j) > 2^{k(k-1)+1-(j-2)}r. \tag{1}$$

For $j \leq k(k-1)+1$, this implies $d^{\mathcal{B}}(c_i, c_j) > 4r$. Since there are at most $k(k-1)$ elements of C of pairwise distance greater than $4r$, this guarantees that $l \leq k(k-1)$. (1) also guarantees that for $1 \leq i < j \leq l$ we have $d^{\mathcal{B}}(c_i, c_j) > 2^{k(k-1)+1-(l-2)}r = 2^{p+1}r$.

Since we stopped at $l = i$, for all $c \in C$ there exists an $i \leq l$ such that $d^{\mathcal{B}}(c, c_i) \leq 2^{k(k-1)+1-(l-1)} = 2^p r$. This proves the claim.

Step 3. Let $p, l, c_1, \ldots, c_l$ be as stated in the claim in Step 2. For $I \subseteq K$, let

$$\varphi_I := \exists x_1 \ldots \exists x_k \Big(\bigwedge_{\substack{i,j \in I \\ i<j}} d(x_i, x_j) > 2^{p+1}r \wedge \bigwedge_{i \in I} \psi_I(x_i) \Big).$$

Since $\mathcal{A} \models \varphi$, we have $\mathcal{A} \models \varphi_I$. Thus, since φ_I is an existential local sentence of rank at most $(k \cdot (w+1), 2^{k^2}r)$, we also have $\mathcal{B} \models \varphi_I$.

Step 4. Let $L := \{1, \ldots, l\}$. We define a relation $R \subseteq K \times L$ as follows: For $i \in K, j \in L$ we let iRj if there is a $b \in B$ such that $\mathcal{B} \models \psi_i(b)$ and $d^{\mathcal{B}}(b, c_j) \leq 2^p r$.

Claim: For every $I \subseteq K$ the set $R(I) := \{j \in L \mid \exists i \in I : iRj\}$ contains at least as many elements as I.

Proof: Recall that $\mathcal{B} \models \varphi_I$. For $i \in I$, let $b_i \in B$, such that for all $i, j \in I$ with $i < j$ we have $d^{\mathcal{B}}(b_i, b_j) > 2^{p+1}r$ and for all $i \in I$ we have $\mathcal{B} \models \psi_I(b_i)$. Then $b_i \in C$, and thus there exist a $j \in L$ such that $d^{\mathcal{B}}(b_i, c_j) \leq 2^p r$. Since $d^{\mathcal{B}}(b_i, b_j) > 2^{p+1} r$, for every $j \in L$ there can be at most one $i \in I$ such that $d^{\mathcal{B}}(b_i, c_j) \leq 2^p r$. This proves the claim.

By the marriage theorem, there exists a one-to-one mapping f of K into L such that for all $i \in K$ we have $iRf(i)$. In other words, there exist $b_1, \ldots, b_k$ such that for $1 \leq i \leq k$ we have $\mathcal{B} \models \psi_i(b_i)$ and $d^{\mathcal{B}}(b_i, c_{f(i)}) \leq 2^p r$. Since $d^{\mathcal{B}}(c_{f(i)}, c_{f(j)}) > 2^{p+1} r$, the latter implies $d^{\mathcal{B}}(b_i, b_j) > 2r$. Thus

$$\mathcal{B} \models \exists x_1 \ldots \exists x_k \Big(\bigwedge_{1 \leq i < j \leq k} d(x_i, x_j) > 2r \wedge \bigwedge_{i=1}^{k} \psi_i(x_i) \Big).$$

$\square$

Lemma 5. *There is a function $f(k)$, such that the following holds for all $k \geq 1$: Let $\mathcal{A}$, $\mathcal{B}$ be structures such that every existential local sentence of rank $(k(k+1), f(k))$ that holds in $\mathcal{A}$ also holds in $\mathcal{B}$. Then every existential sentence of weight at most k that holds in $\mathcal{A}$ also holds in $\mathcal{B}$.*

Proof: Since every existential sentence is equivalent to a disjunction of conjunctive queries with negation of the same weight, it suffices to prove that every conjunctive query with negation of weight k that holds in $\mathcal{A}$ also holds in $\mathcal{B}$. Let

$$\varphi := \exists x_1 \ldots \exists x_k \psi(x_1, \ldots, x_k)$$

with

$$\psi(x_1, \ldots, x_k) := \Big(\bigwedge_{i=1}^{p} \alpha_i \wedge \bigwedge_{i=1}^{q} \beta_i \Big),$$

where all the α_i are atoms and the β_i are negated atoms. Suppose that $\mathcal{A} \models \varphi$. We shall prove that $\mathcal{B} \models \varphi$.

We define the *positive graph of* φ to be the graph $\mathcal{G}$ with universe $G := \text{var}(\varphi) = \{x_1, \ldots, x_k\}$ and

$$E^{\mathcal{G}} := \{xy \mid \exists i, 1 \leq i \leq p : \ x, y \in \text{var}(\alpha_i)\}.$$

Let $\mathcal{H}_1, \ldots, \mathcal{H}_r$ be the connected components of $\mathcal{G}$. Without loss of generality, we may assume that for $1 \leq i \leq r$ we have $x_i \in H_i$. Then we know that $H_i \subseteq N_k^{\mathcal{G}}(x_i)$. If $r = 1$, then this means that $\text{var}(\varphi) \subseteq N_k^{\mathcal{G}}(x_1)$, and φ is equivalent to the k-local sentence

$$\exists x_1 \, \exists x_2 \in N_k(x_1) \ldots \exists x_k \in N_k(x_1) \psi$$

of rank (k, k). If we choose f such that $f(k) \geq k$, then $\mathcal{A} \models \varphi$ implies $\mathcal{B} \models \varphi$. In the following, we assume that $r \geq 2$.

Let $c_0 := 0$ and $c_{i+1} := 2^{k^2}(c_i + k + 1)$ for $i \geq 0$. We let $R := \big\{\{i, j\} \bigm| 1 \leq i < j \leq r\big\}$, $h := |R| = \binom{r}{2}$ and

$$f(k) = 2^{k^2}(c_h + k + 1). \tag{2}$$

For $\bar{a} = a_1 \dots a_r \in A^r$, the *distance pattern* of $\bar{a}$ is the mapping $\Delta_{\bar{a}} : R \to \{0, \dots, h\}$ defined by

$$\Delta_{\bar{a}}(\{i,j\}) := \begin{cases} 0 & \text{if } d^{\mathcal{A}}(a_i, a_j) = 0 \\ t & \text{if } c_t < d^{\mathcal{A}}(a_i, a_j) \le c_{t+1} \text{ for some } t \text{ such that } 0 \le t < h \\ h & \text{if } d^{\mathcal{A}}(a_i, a_j) > c_h \end{cases}$$

By the pigeonhole principle, for every distance pattern Δ there is an integer $\text{gap}(\Delta)$ such that $0 \le \text{gap}(\Delta) \le h$ and $\Delta(\{i,j\}) \ne \text{gap}(\Delta)$ for all $\{i,j\} \in R$.

Let $\bar{a} = a_1 \dots a_k \in A^k$ such that $\mathcal{A} \models \psi(\bar{a})$. Let $\Delta := \Delta_{a_1 \dots a_r}$, and $g := \text{gap}(\Delta)$. Then for all $\{i,j\} \in R$ we either have $d(a_i, a_j) \le c_g$ or $d(a_i, a_j) > 2^{k^2}(c_g + k + 1)$. This implies that the relation on $\{a_1, \dots, a_r\}$ defined by $d^{\mathcal{A}}(a_i, a_j) \le c_g$ is an equivalence relation. Without loss of generality, we may assume that $a_1, \dots, a_s$ form a system of representatives of the equivalence classes.

We let $l := c_g + k$. For $1 \le i \le s$, we let $I_i := \{j \mid 1 \le j \le k, d^{\mathcal{A}}(a_i, a_j) \le l\}$. Then $(I_i)_{1 \le i \le s}$ is a partition of $\{1, \dots, k\}$. To see this, first recall that for $1 \le j \le r$ there is an $i, 1 \le i \le s$ such that $d^{\mathcal{A}}(a_i, a_j) \le c_g$. For t with $r+1 \le t \le k$ there exist a $j, 1 \le j \le r$ such that $x_t \in H_j$, the connected component of x_j in the positive graph of φ. Since $\mathcal{A} \models \psi(\bar{a})$, this implies that $d^{\mathcal{A}}(a_j, a_t) \le k$. Thus there exists an $i, 1 \le i \le s$ such that $d^{\mathcal{A}}(a_i, a_t) \le c_g + k$.

For $1 \le i \le s$, we let

$$\psi_i(x_i) := \exists \bar{x}^i \in N_l(x_i) \bigwedge_{\text{var}(\alpha_i) \subseteq I_i} \alpha_i \wedge \bigwedge_{\text{var}(\beta_i) \subseteq I_i} \beta_i,$$

where $\bar{x}^i$ consists of all variables x_j with $j \in I_i \setminus \{i\}$. Then for $1 \le i \le s$ we have $\mathcal{A} \models \psi_i(a_i)$, because $\mathcal{A} \models \psi(\bar{a})$. Thus

$$\mathcal{A} \models \exists x_1 \dots \exists x_s \Big(\bigwedge_{1 \le i < j \le s} d(x_i, x_j) > 2^{k^2}(l+1) \wedge \bigwedge_{1 \le i \le s} \psi_i(x_i) \Big).$$

Since $f(k) = 2^{k^2}(c_h + k + 1) \ge 2^{k^2}(l+1)$, by Lemma 4, this implies

$$\mathcal{B} \models \exists x_1 \dots \exists x_s \Big(\bigwedge_{1 \le i < j \le k} d(x_i, x_j) > 2(l+1) \wedge \bigwedge_{1 \le i \le s} \psi_i(x_i) \Big).$$

Thus there exist $b_1, \dots, b_s \in B$ such that for $1 \le i < j \le s$ we have $d^{\mathcal{B}}(b_i, b_j) > 2(l+1)$ and for $1 \le i \le s$ we have $\mathcal{B} \models \psi_i(b_i)$. Since $I_1, \dots, I_s$ is a partition of $\{1, \dots, k\}$, there are $b_{s+1}, \dots, b_k \in B$ such that:

(i) $d^{\mathcal{B}}(b_i, b_j) \le l$ for all $j \in I_i$.

(ii) $\mathcal{B} \models \alpha_j(\bar{b})$ for all $j, 1 \le j \le p$ such that $\text{var}(\alpha_j) \subseteq I_j$.

(iii) $\mathcal{B} \models \beta_j(\bar{b})$ for all $j, 1 \le j \le q$ such that $\text{var}(\beta_j) \subseteq I_j$.

We claim that $\mathcal{B} \models \psi(\bar{b})$. Since for each connected component H_j of the positive graph of φ there is an $i, 1 \le i \le s$ such that $t \in I_i$ whenever $x_t \in H_j$, (ii) implies that

$\mathcal{B} \models \alpha_j(\bar{b})$ for $1 \leq j \leq p$. It remains to prove that $\mathcal{B} \models \beta_j(\bar{b})$ for $1 \leq j \leq q$. If $\text{var}(\beta_j) \subseteq I_i$ for some i, then $\mathcal{B} \models \beta_j(\bar{b})$ by (iii). Otherwise, β_j has variables x_u, x_v such that there exist $i \neq i'$ with $x_u \in I_i, x_v \in I_{i'}$. Then by (i), $d^{\mathcal{B}}(b_i, b_u) \leq l$ and $d^{\mathcal{B}}(b_{i'}, b_v) \leq l$. Since $d^{\mathcal{B}}(b_i, b_{i'}) > 2l + 1$, this implies $d^{\mathcal{B}}(b_u, b_v) > 1$. Since β_j is a negated atom, this implies $\mathcal{B} \models \beta_j(\bar{b})$.

Thus $\mathcal{B} \models \varphi$. $\square$

Proof (of Theorem 2): Let φ be an existential sentence of weight k and $\mathcal{K} := \{\mathcal{A} | \mathcal{A} \models \varphi\}$ the class of all finite structures satisfying φ. Let Ψ be the set of all existential local sentences of rank at most $(k(k+1), f(k))$, where f is the function from Lemma 5. Let

$$\varphi' := \bigvee_{\mathcal{A} \in \mathcal{K}} \bigwedge_{\substack{\psi \in \Psi \\ \mathcal{A} \models \psi}} \psi.$$

We claim that φ is equivalent to φ'. The forward implication is trivial, and the backward implication follows from Lemma 5. Since up to logical equivalence, the set Ψ is finite and therefore φ' contains at most $2^{|\Psi|}$ non-equivalent disjuncts, this proves the theorem. $\square$

Our proof of the existential version of Gaifman's theorem does not give us good bounds on the size and rank of the local formulas to which we translate a given existential formula. Therefore, for the algorithmic applications, it is preferable to work with the following weaker version of Theorem 2, which gives us better bounds.

An *asymmetric local sentence* is a sentence φ of the form

$$\exists x_1 \ldots \exists x_k \Big(\bigwedge_{1 \leq i < j \leq k} d(x_i, x_j) > 2r \wedge \bigwedge_{1 \leq i \leq k} \psi_i(x_i) \Big),$$

where $r, k \geq 1$ and $\psi_1(x), \ldots, \psi_k(x)$ are r-local. φ is an *existential asymmetric local sentence*, if in addition $\psi_1(x), \ldots, \psi_k(x)$ are existential.

An *r-local conjunctive query with negation*, for some $r \geq 1$, is a formula $\psi(x)$ of the form $\exists y_1 \in N_r(x) \ldots \exists y_n \in N_r(x) \bigwedge_{i=1}^m \lambda_i$, where each λ_i is a literal.

Theorem 6. *Every existential first-order sentence φ is equivalent to a disjunction φ' of existential asymmetric local sentences.*

More precisely, if k is the weight of φ and l its size, then φ' is a disjunction of $2^{O(l+k^4)}$ asymmetric local sentences of the form

$$\exists x_1 \ldots \exists x_k \Big(\bigwedge_{1 \leq i < j \leq k} d(x_i, x_j) > 2r \wedge \bigwedge_{1 \leq i \leq k} \psi_i(x_i) \Big),$$

where $\psi_1, \ldots, \psi_k$ are r-local conjunctive queries with negation. The rank of each of these local sentences is at most $(k, 2^{k^2+1})$, and their size is in $O(l)$.

Furthermore, there is a polynomial p and an algorithm translating φ to φ' in time $O(2^{p(l)})$.

Proof: We first assume that φ is a conjunctive query with negation, say,

$$\varphi := \exists x_1 \ldots \exists x_k \psi(x_1, \ldots, x_k)$$

with

$$\psi(x_1, \ldots, x_k) := \Big(\bigwedge_{i=1}^{p} \alpha_i \wedge \bigwedge_{i=1}^{q} \beta_i \Big),$$

where all the α_i are atoms and the β_i are negated atoms. Without loss of generality, we may assume that $k \geq 2$, because for $k = 1$ there is nothing to prove. We define the *positive graph of* φ to be the graph $\mathcal{G}$ with $G := \text{var}(\varphi) = \{x_1, \ldots, x_k\}$ and

$$E^{\mathcal{G}} := \{xy \mid \exists i, 1 \leq i \leq p : \ x, y \in \text{var}(\alpha_i)\}.$$

Let $\mathcal{H}_1, \ldots, \mathcal{H}_r$ be the connected components of $\mathcal{G}$. Without loss of generality, we may assume that $r \geq 2$, and that for $1 \leq i \leq r$ we have $x_i \in H_i$. Then we know that $H_i \subseteq N_k^{\mathcal{G}}(x_i)$.

Let $c_0 := 0$ and $c_{i+1} := 2(c_i + k + 1)$ for $i \geq 0$. Let $R := \big\{\{i, j\} \bigm| 1 \leq i < j \leq r\big\}$ and $h := |R| = \binom{r}{2}$. It is not difficult to prove that $c_h + k + 1 \leq 2^{k^2+1}$.

Let $\mathcal{A}$ be a structure and $\bar{a} = a_1 \ldots a_r \in A^r$. The *distance pattern* of $\bar{a}$ is the mapping

$$\Delta_{\bar{a}} : R \to \{0, \ldots, h\}$$

defined by

$$\Delta_{\bar{a}}(\{i,j\}) := \begin{cases} 0 & \text{if } d^{\mathcal{A}}(a_i, a_j) = 0 \\ t & \text{if } c_t < d^{\mathcal{A}}(a_i, a_j) \leq c_{t+1} \text{ for some } t \text{ such that } 0 \leq t < h \\ h & \text{if } d^{\mathcal{A}}(a_i, a_j) > c_h \end{cases}$$

By the pigeonhole principle, for every distance pattern Δ there is a number $\text{gap}(\Delta), 0 \leq \text{gap}(\Delta) \leq h$ such that $\Delta(\{i,j\}) \neq \text{gap}(\Delta)$ for all $\{i,j\} \in R$.

Let $\bar{a} \in A^r$, $\Delta := \Delta_{\bar{a}}$, and $g := \text{gap}(\Delta)$. Then for all $\{i,j\} \in R$ we either have $d(a_i, a_j) \leq c_g$ or $d(a_i, a_j) > 2(c_g + k + 1)$. This implies that the relation on $\{a_1, \ldots, a_r\}$ defined by $d^{\mathcal{A}}(a_i, a_j) \leq c_g$ is an equivalence relation. Without loss of generality, we may assume that $a_1, \ldots, a_s$ form a system of representatives of the equivalence classes.

Now suppose that we extend $a_1 \ldots a_r$ to a k-tuple $\bar{a} = a_1 \ldots a_k \in A^k$ such that $\mathcal{A} \models \psi(\bar{a})$. We let $l := c_g + k$. For $1 \leq i \leq s$, we let $I_i := \{j \mid d^{\mathcal{A}}(a_i, a_j) \leq l\}$. Then $(I_i)_{1 \leq i \leq s}$ is a partition of $\{1, \ldots, k\}$. For $1 \leq i \leq s$, we let

$$\psi_i(x_i) := \exists \bar{x}^i \in N_l(x_i) \bigwedge_{\text{var}(\alpha_i) \subseteq I_i} \alpha_i \wedge \bigwedge_{\text{var}(\beta_i) \subseteq I_i} \beta_i,$$

where $\bar{x}^i$ consists of all variables x_j with $j \in I_i \setminus \{i\}$, and

$$\psi_\Delta(x_1, \ldots, x_s) := \bigwedge_{1 \leq i < j \leq s} d(x_i, x_j) > 2(l+1) \wedge \bigwedge_{1 \leq i \leq s} \psi_i(x_i).$$

Then $\mathcal{A} \models \psi_\Delta(a_1, \ldots, a_s)$. Furthermore, for every tuple $a'_1 \ldots a'_s \in A^s$ with $\mathcal{A} \models \psi_\Delta(a'_1, \ldots, a'_s)$ there exists an extension $\bar{a}' := a'_1 \ldots a'_k$ such that $\mathcal{A} \models \psi(\bar{a}')$. To see this, observe that every positive literal α_j occurs in an I_i and thus in ψ_Δ, and every negative literal β_j either occurs in an I_i or has variables with indices in two distinct $I_i, I_{i'}$ and is thus automatically satisfied, because the variables are forced to be far apart.

The formula $\psi_\Delta(x_1, \dots, x_k)$ only depends on the distance pattern Δ and not on the tuple $\bar{a}$ realizing it. So for every distance pattern Δ we obtain a formula $\psi_\Delta(\bar{x}^\Delta)$, whose free variables $\bar{x}^\Delta$ are among $x_1, \dots, x_r$, with the following properties:

- $\exists \bar{x}^\Delta \psi_\Delta$ is an existential asymmetric local sentence of rank at most $(k, 2^{k^2+1})$.
- For every tuple $\bar{a} \in A^k$ with $\mathcal{A} \models \psi(\bar{a})$ and $\Delta_{\bar{a}} = \Delta$ we have $\mathcal{A} \models \psi_\Delta(\bar{a}^\Delta)$, where $\bar{a}^\Delta$ consists of the same entries of $\bar{a}$ as $\bar{x}^\Delta$ of $\bar{x}$.
- Every tuple $\bar{a}^\Delta$ with $\mathcal{A} \models \psi_\Delta(\bar{a}^\Delta)$ can be extended to a tuple $\bar{a} = a_1 \dots a_k$ such that $\mathcal{A} \models \psi(\bar{a})$.

The last two items imply that φ is equivalent to the formula

$$\varphi' := \bigvee_{\Delta \text{ distance pattern}} \exists \bar{x}^\Delta \psi_\Delta.$$

It is not hard to see that the number of distance pattern is in $2^{O(k^4)}$, thus φ is a disjunction of $2^{O(k^4)}$ existential asymmetric local sentences of rank at most $(k, 2^{k^2+1})$ and size in $O(l)$ (where l denotes the length of φ).

If φ is an arbitrary existential sentence, we first transform it to a disjunction of at most 2^l conjunctive queries with negation of the same weight as φ.

Finally, we observe that the translation from φ to the disjunction of asymmetric local formulas is effective within the desired time bound: Given φ, we first translate it to a disjunction of conjunctive queries with negation. This is possible in time $2^{O(l)}$. Then we treat each of the conjunctive queries with negation separately. We compute the positive graph and all possible patterns. For each of pattern Δ, we compute the gap and then the formula φ_Δ. Since $k \leq l$, this is clearly possible in time $2^{p(l)}$ for a suitable polynomial p. □

4 An Algorithmic Application

The appropriate structural notion for the algorithmic applications of locality is *bounded local tree-width*. We assume that the reader is familiar with the definition of *tree-width* of graphs (see e.g. [4]). The tree-width of a structure $\mathcal{A}$, denoted by $\mathrm{tw}(\mathcal{A})$, is the tree-width of its Gaifman graph. The *local tree-width* of a structure $\mathcal{A}$ is the function $\mathrm{ltw}_\mathcal{A} : \mathbb{N} \to \mathbb{N}$ defined by

$$\mathrm{ltw}_\mathcal{A}(r) := \max\Big\{ \mathrm{tw}\big(\langle N_r^\mathcal{A}(a)\rangle\big) \;\Big|\; a \in A \Big\}.$$

A class C of structures has *bounded local tree-width* if there is a function $\lambda : \mathbb{N} \to \mathbb{N}$ such that $\mathrm{ltw}_\mathcal{A}(r) \leq \lambda(r)$ for all $\mathcal{A} \in \mathrm{C}, r \in \mathbb{N}$. Many well-known classes of structures have bounded local tree-width, among them the class of planar graphs and all classes of structures of bounded degree.

Theorem 7 (Frick and Grohe [11]). *Let* C *be a class of structures of bounded local tree-width. Then there is a function f and, for every $\epsilon > 0$, an algorithm deciding in time $O(f(||\varphi||)|A|^{1+\epsilon})$ whether a given structure $\mathcal{A} \in$ C satisfies a given first-order sentence φ.*

If the class C is *locally tree-decomposable*, which is a slightly stronger requirement than having bounded local tree-width, then there is a function f and an algorithm deciding whether a given structure $\mathcal{A} \in$ C satisfies a given first-order sentence φ in time $O(f(||\varphi||)|A|)$.

These algorithms proceed as follows: Given a structure $\mathcal{A}$ and a sentence φ, they first translate φ to a Boolean combination of local sentences. Then they evaluate each local sentence and combine the results. To evaluate a local sentence, say,

$$\exists x_1 \ldots \exists x_k \Big(\bigwedge_{1 \leq i < j \leq k} d(x_i, x_j) > 2r \wedge \bigwedge_{1 \leq i \leq k} \psi(x_i) \Big),$$

they first compute the set $\psi(\mathcal{A})$ of all $a \in A$ such that $\mathcal{A} \models \psi(a)$. Since ψ is local and the class C has bounded local tree-width or even is locally tree-decomposable, this is possible quite efficiently. (In the special case of structures of bounded degree, this is easy to see, because ψ only has to be evaluated in substructures of $\mathcal{A}$ of bounded size.) Finally, the algorithms test whether there are $a_1, \ldots, a_k \in \psi(\mathcal{A})$ of pairwise distance greater than $2r$. This is possible in linear time by the following lemma:

Lemma 8 (Frick and Grohe [11]). *Let* C *be a class of structures of bounded local tree-width. Then there is a function g and an algorithm that, given a structure $\mathcal{A}$, a subset $P \subseteq A$, and integers k, r, decides in time $O(g(k,r)|A|)$ whether there are $a_1, \ldots, a_k \in P$ of pairwise distance greater than $2r$.*

The drawback of these algorithms is that we cannot even give an elementary upper bound for the function f in Theorem 7. The main reason for the enormous runtime of the algorithms in terms of the formula size is that to evaluate the local formulas, they translate them to tree-automata, and in the worst case the size of these automata grows exponentially with each quantifier alternation. Therefore, it is a natural idea to bound the number of quantifier alternations in order to obtain smaller automata. But this would require that the translation of first-order sentences into local sentences preserves the quantifier structure. Unfortunately, the known proofs of Gaifman's theorem do not preserve the quantifier structure of the input formula.

These considerations motivated the present paper. Indeed, Theorem 2 shows that existential first-order sentences can be translated into Boolean combinations of existential local formulas. The price we pay for this is that these Boolean combinations of existential local formulas can get enormously large. Therefore, we use Theorem 6, because this theorem at least gives us an exponential upper bound on the size of the resulting formula. To evaluate an asymmetric local sentence, say

$$\exists x_1 \ldots \exists x_k \Big(\bigwedge_{1 \leq i < j \leq k} d(x_i, x_j) > 2r \wedge \bigwedge_{1 \leq i \leq k} \psi_i(x_i) \Big),$$

where the ψ_i are conjunctive queries with negation, we first compute the sets $\psi_1(\mathcal{A})$, …, $\psi_k(\mathcal{A})$. This can be done as in the algorithms described above, but is actually faster since the ψ_i are conjunctive queries with negation. We use Lemma 9. Then we have to decide whether there are $a_1 \in \psi_1(\mathcal{A}), \dots, a_k \in \psi_k(\mathcal{A})$ of pairwise distance greater than $2r$. Lemma 10 is an analogue of Lemma 8 for this more general situation.

Lemma 9. *There is a polynomial p and an algorithm that solves the following problem in time $O(2^{p(||\varphi||+\mathrm{tw}(\mathcal{A}))} \cdot |A|)$.*

Input:	Structure $\mathcal{A}$, conjunctive query with negation φ.
Problem:	Decide if $\mathcal{A} \models \varphi$.

Details of the proof of Lemma 9 and the following Lemma 10 can be found in the full version of this paper [13] and in the second author's Diploma thesis [21].

Lemma 10. *There is a polynomial p and an algorithm that solves the following problem in time $O(2^{p(\mathrm{ltw}_{\mathcal{A}}((k+1)r)+r+k)} \cdot |A|)$:*

Input:	Structure $\mathcal{A}$, sets $P_1, \dots, P_k \subseteq A$, integer $r \geq 1$.
Problem:	Decide if there are $a_1 \in P_1, \dots, a_k \in P_k$ of pairwise distance greater than k.

If we combine these two lemmas together with Theorem 6 and plug them in the algorithms described in [11], we obtain the following theorem.

Theorem 11. *Let* C *be a class of structures whose local tree-width is bounded by a function $\lambda : \mathbb{N} \to \mathbb{N}$ (i.e., for all $\mathcal{A} \in$ C and $r \geq 0$ we have $\mathrm{ltw}_{\mathcal{A}}(r) \leq \lambda(r)$). Then there are polynomials p, q such that for every $\epsilon > 0$ there is an algorithm that, given a structure $\mathcal{A}$ and an existential first-order sentence φ, decides if $\mathcal{A} \models \varphi$ in time*

$$O\left(2^{2^{p(\lambda(q(||\varphi||+(1/\epsilon)))+||\varphi||+(1/\epsilon))}} \cdot |A|^{1+\epsilon}\right),$$

i.e., in time doubly exponential in $||\varphi||, (1/\epsilon), \lambda(q(||\varphi|| + (1/\epsilon)))$ and near linear in $|A|$.

For many interesting classes of structures of bounded local tree-width, such as planar graphs, the local tree-width is bounded by a linear function λ.

5 Conclusions

Our main result is an existential version of Gaifman's locality theorem. It would be interesting to see if there are similar structure preserving locality theorems for other classes of first-order formulas, such as formulas monotone in some relation symbol or Σ_2-formulas. The combinatorial techniques we use in our proof seem to be specific to existential formulas; we do not see how to apply them to other classes of formulas. With the algorithmic applications in mind, it would be nice to get better bounds on the size and rank of the Boolean combinations of local sentences the locality theorems give us, both in the existential and in the general case.

In the second part of the paper, we show how a variant of our locality theorem can be applied to evaluate existential first-order sentences in structures of bounded local tree-width by improving an algorithm of [11] for the special case of existential sentences. We are able to prove a doubly exponential upper bound for the dependence of the runtime of the algorithm on the size of the input sentence. Though not really convincing, it is much better than what we have for arbitrary first-order sentences — recall that no elementary bound is known there — and it shows that quantifier alternation really is an important factor contributing to the large complexity. It might be possible to further improve the algorithm to obtain a (singly) exponential dependence on the size of the input sentence. But even then we would probably not get a practical algorithm, because the hidden constant would still be too large.

The best chance to get practical algorithms might be to concentrate on particular classes of graphs, such as graphs of bounded degree or planar graphs, and use their specific properties. For example, the local tree-width of planar graphs is bounded by the function $r \mapsto 3 \cdot r$, and it is quite easy to compute tree-decompositions of neighborhoods in planar graphs [2, 9]. This already eliminates certain very expensive parts of our algorithms. The algorithms can also be improved by using weaker forms of locality. We have taken a step in this direction by admitting asymmetric local sentences. Further improvement might be possible by admitting "weak" asymmetric sentences stating that there are elements of pairwise distance greater than s satisfying some r-local condition, where s is no longer required to be $2r$. For the algorithms, it does not really matter if the local neighborhoods are disjoint, and relaxing this condition may give us smaller formulas.

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