SEMANTIC TREE-WIDTH AND PATH-WIDTH OF CONJUNCTIVE REGULAR PATH QUERIES*

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ABSTRACT. We show that the problem of whether a query is equivalent to a query of tree-width k is decidable, for the class of Unions of Conjunctive Regular Path Queries with two-way navigation (UC2RPQs). A previous result by Barceló, Romero, and Vardi [BRV16] has shown decidability for the case k=1, and here we extend this result showing that decidability in fact holds for any arbitrary $k \ge 1$. The algorithm is in 2ExpSpace, but for the restricted but practically relevant case where all regular expressions of the query are of the form a^* or $(a_1 + \cdots + a_n)$ we show that the complexity of the problem drops to Π_p^p .

We also investigate the related problem of approximating a UC2RPQ by queries of small tree-width. We exhibit an algorithm which, for any fixed number k, builds the maximal under-approximation of tree-width k of a UC2RPQ. The maximal under-approximation of tree-width k of a query q is a query q' of tree-width k which is contained in q in a maximal and unique way, that is, such that for every query q'' of tree-width k, if q'' is contained in q then q'' is also contained in q'.

Our approach is shown to be robust, in the sense that it allows also to test equivalence with queries of a given path-width, it also covers the previously known result for k=1, and it allows to test for equivalence of whether a (one-way) UCRPQ is equivalent to a UCRPQ of a given tree-width (or path-width).

This pdf contains internal links: clicking on a notion leads to its definition.

 $^{^{1}\}mathrm{This}$ result was achieved by using the <code>knowledge</code> package and its companion tool <code>knowledge-clustering</code>.



Key words and phrases: graph databases, conjunctive regular path queries, semantic optimization, treewidth, path-width, containment, approximation.

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Contents

1. Introduction	3
1.1. Graph Databases	3
1.2. Related Work	7
1.3. Contributions	8
1.4. Conference Paper	11
2. Preliminaries	11
3. Maximal Under-Approximations	15
4. Intermezzo: Tagged Tree Decompositions	19
5. Key Lemma: Maximal Under Approximations are Semantically Finite	24
5.1. Local Acyclicity	24
5.2. Short Paths	27
5.3. Proof of Lemma 3.8	32
6. Semantic Tree-Width for Simple Queries	32
6.1. Summary Queries	33
6.2. Semantic Tree-Width Problem	35
7. Acyclic Queries: the Case $k=1$	37
7.1. Contracted Tree-Width	37
7.2. The Key Lemma for Contracted Tree-Width One	39
8. Semantic Path-Width	41
8.1. Path-Width of Queries	41
8.2. Deciding Bounded Semantic Path-Width	42
8.3. Evaluation of Queries of Bounded Semantic Path-Width	45
9. Lower Bounds for Deciding Semantic Tree-Width and Path-Width	47
10. Discussion	49
10.1. Complexity	49
10.2. Characterization of Tractability	50
10.3. Larger Classes	53
10.4. Different Notions	53
Appendix A. Polynomial-Time Evaluation of Queries of Bounded Tree-Width	55
Appendix B. Alternative Upper Bound for Containment of UC2RPQs	56
Appendix C. Path-Width is not Closed under Refinements	57
Acknowledgment	58
References	58

1. Introduction

1.1. **Graph Databases.** Graph databases have gained significant attention due to their ability to efficiently model and manage complex, interconnected data. Unlike traditional relational databases, they model data as entities connected by edges that represent relationships. This structure facilitates the analysis of highly interconnected data, where the topology of the connections is as crucial as the data itself, making them particularly well-suited for use cases like biology, social networks, banking, recommendation systems, and fraud detection. We refer the reader to [Bar13, Woo12, AAB⁺17] for surveys on the foundations and applications of graph databases.

Graph databases are abstracted as edge-labelled directed graphs $G = \langle V(G), E(G) \rangle$, where nodes of V(G) represent entities and labelled edges $E(G) \subseteq V(G) \times \mathbb{A} \times V(G)$ represent relations between these entities, with \mathbb{A} being a fixed finite alphabet. For instance, Figure 1 depicts a graph database, whose nodes are authors and papers, on the alphabet $\mathbb{A} = \{\text{wrote}, \text{advised}\}$. Edges $x \xrightarrow{\text{wrote}} y$ indicate that the person x wrote the paper y, while edges $x \xrightarrow{\text{advised}} y$ indicate that person x was the Ph.D. advisor of person y.



FIGURE 1. A graph database with eight nodes and eight edges on a two-letter alphabet.

Being a subclass of relational databases, graph databases can be queried by the predominant query language of *conjunctive queries*, also known as CQs, which consists of the closure under projection—also known as existential quantification—of conjunctions of atoms of the form $x \stackrel{a}{\to} y$ for some letter $a \in A$. For instance, the conjunctive query

$$\gamma_1(x,y) = x \xrightarrow{\text{wrote}} z \land y \xrightarrow{\text{wrote}} z$$

returns, when evaluated on the graph database G defined in Figure 1, all pairs of nodes (u,v) such that u is a co-author of v. Each variable not appearing in the left-hand side of the definition of a conjunctive query (in this example, z) is implicitly existentially quantified. Note that, to the cost of losing the information of which variable is existentially quantified, every CQ can be seen as a graph database, where each variable is a node, and each atom is an edge; hence, we sometimes use graph database terminology for CQs.

The expressive power of CQs is somewhat limited, since CQs cannot express, for example, transitive closure. Since the ability to navigate paths is of importance in many graph database scenarios, most modern graph query languages support, as a central querying mechanism, conjunctive regular path queries, or CRPQs for short. In particular, CRPQs form the core navigational mechanism of the new ISO standard Graph Query Language (GQL) [ISO24a] and the SQL extension for querying graph-structured data SQL/PGQ [ISO24b] (see also [FGG⁺23b, FGG⁺23a]).

CRPQs are defined analogously to conjunctive queries, except that their atoms are now of the form $x \xrightarrow{L} y$ where L is an arbitrary regular language over the alphabet \mathbb{A} . For instance the evaluation of the CRPQ

$$\gamma_2(x,y) = x \xrightarrow{\text{wrote}} z \wedge z' \xrightarrow{\text{wrote}} z \wedge y \xrightarrow{\text{(advised)}^*} z'$$

on G yields every pair of persons (u, v) such that u is a co-author of a "scientific descendant" of v.

Formally, a CRPQ γ is defined as a tuple $\bar{z}=(z_1,\ldots,z_n)$ of $output\ variables$, also known as $free\ variables$, 2 together with a conjunction of atoms of the form $\bigwedge_{j=1}^m x_j \xrightarrow{L_j} y_j$, where each L_j is a regular language and where $m \geq 0$. The set of all variables occurring in γ , namely 3 $\{z_1,\ldots,z_n\} \cup \{x_1,y_1,\ldots,x_m,y_m\}$, is denoted by $vars(\gamma)$. Given a database G, we say that a tuple of nodes $\bar{u}=(u_1,\ldots,u_n)$ satisfies γ on G if there is a mapping $f\colon vars(\gamma) \to V(G)$ such that $u_i=f(z_i)$ for all $1 \leq i \leq n$, and for each $1 \leq j \leq m$, there exists a path from $f(x_i)$ to $f(y_i)$ in G, labelled by a word from L_i (if the path is empty, the label is ε). The evaluation of γ on G is then the set of all tuples that satisfy γ . For example, (author₂, author₅) satisfies γ_2 on the graph database G of Figure 1 via the function that maps x to author₂, y to author₅, z to paper₂, and z' to author₃.

The language of CRPQ can be extended to navigate edges in both directions. Consider the expanded database G^{\pm} obtained from G by adding, for every edge $x \xrightarrow{a} y$ in G, an extra edge $y \xrightarrow{a^-} x$. We obtain a graph database on the alphabet $\mathbb{A}^{\pm} = \mathbb{A} \cup \mathbb{A}^-$ where $\mathbb{A}^- = \{a^- \mid a \in \mathbb{A}\}$. We then define the syntax of a CRPQ with two-way navigation, or C2RPQ, as a CRPQ on the alphabet \mathbb{A}^{\pm} . Its evaluation is defined as the evaluation of the CRPQ on G^{\pm} . For instance, the evaluation of the C2RPQ

$$\gamma_3(x,y) = x \xrightarrow{\text{(wrote·wrote^-)*}} y$$

on the graph database of Figure 1 returns all pairs of individuals linked by a chain of coauthorship. It includes (author₁, author₃) or (author₁, author₁) but not (author₁, author₄). If a query has no output variables we call it *Boolean*, and its evaluation can either be the set $\{()\}$, in which case we say that G satisfies the query, or the empty set $\{\}$. For example, G satisfies the Boolean CRPQ

$$\gamma_4() = x \xrightarrow{\text{wrote}} y$$

if, and only if, the database contains one author together with one paper they wrote.

To simplify proofs, we assume that all the regular languages are described via non-deterministic finite automata (NFA) instead of regular expressions, which does not affect any of our complexity bounds. However, for readability all our examples will be given in terms of regular expressions. We denote the set of atoms of a C2RPQ γ by Atoms(γ), and by $\|\gamma\|_{at}$ we denote its number of atoms, *i.e.*, |Atoms(γ)|. Moreover, we denote by $\|\gamma\|$ the sum of its number of atoms with the sum of the size of NFAs used to describe γ .

Finally, a union of CQs (UCQs) (resp. union of CRPQs (UCRPQs), resp. union of C2RPQs (UC2RPQs)) is defined as a finite set of CQs (resp. CRPQs, resp. C2RPQs), whose tuples of output variables have all the same arity. A subquery of a C2RPQ γ is any C2RPQ resulting from removing some atoms (possibly none) from γ . A subquery of UC2RPQ is a

²For technical reasons (see the definition of equality atoms) we allow for a variable to appear multiple times.

³We neither assume disjointness nor inclusion between $\{z_1,\ldots,z_n\}$ and $\{x_1,y_1,\ldots,x_m,y_m\}$

union of subqueries of the C2RPQs therein. The evaluation of a union is defined as the union of its evaluations, for instance the following UCQ

$$\Gamma_5 = \gamma_5^1(x, y) \vee \gamma_5^2(x, y)$$
where $\gamma_5^1(x, y) = x \xrightarrow{\text{wrote}} y$ and $\gamma_5^2(x, y) = x \xleftarrow{\text{advised}} z \wedge z \xrightarrow{\text{wrote}} y$

evaluates to the set of pairs (x, y) such that y is a paper written by either x or their advisor. We naturally extend the notations $\|-\|_{\text{at}}$ and $\|-\|$ to unions. *Infinitary unions* are defined analogously, except that we allow for potentially infinite unions. We often use a set notation to denote the union, especially for infinitary unions.

For a more detailed introduction to CRPQs, we refer the reader to [Fig21]. For a more general introduction to different query languages for graph databases—including CRPQs—see [BB13], and for a more practical approach, see [AAB⁺17].

The evaluation problem for UC2RPQ is the problem of, given a UC2RPQ Γ , a graph database G and a tuple \bar{u} of elements of G, whether \bar{u} satisfies Γ on G. Given two UC2RPQ Γ and Γ' whose output variables have the same arity, we say that Γ is contained in Γ' , denoted by $\Gamma \subseteq \Gamma'$ if for every graph database G, for every tuple \bar{u} of G, if \bar{u} satisfies Γ on G, then so does Γ' (we will hence reserve the symbol ' \subseteq ' for set inclusion—note in particular that inclusion (of the UC2RPQs, seen as sets of C2RPQs) implies containment, but the converse does not hold). The containment problem for UC2RPQs is the problem of, given two UC2RPQs Γ and Γ' , to decide if $\Gamma \subseteq \Gamma'$. When Γ is contained in Γ' and vice versa, we say that Γ and Γ' are semantically equivalent, denoted by $\Gamma \equiv \Gamma'$.

Queries of small tree-width. It is known that the evaluation problem for UC2RPQ is NP-complete, just as for conjunctive queries [CM77, Theorem 7]. However, queries whose underlying structure looks like a tree—formally, queries of bounded tree-width—can be evaluated in polynomial time [CR00, Theorem 3].⁴

Tree-width is a measure of how much a graph differs from a tree, introduced by Arnborg, Corneil and Proskurowski [ACP87]. For a gentle but thorough introduction to tree-width, we refer the reader to [NdM12, §3.6]. Formally, a tree decomposition of a multigraph G is a pair (T, \mathbf{v}) where T is a tree and $\mathbf{v} : V(T) \to \mathcal{P}(vars(G))$ is a function that associates to each node of T, called bag, a set of vertices of G. When $x \in \mathbf{v}(b)$ we shall say that the bag $b \in V(T)$ contains vertex v. Further, it must satisfy the following three properties:

- each vertex v of γ is contained in at least one bag of T;
- for each edge $u \to v$ of G, there is at least one bag of T that contains both u and v; and
- for each vertex v of G, the set of bags of T containing v is a connected subset of V(T).

The width of (T, \mathbf{v}) is the maximum of $|\mathbf{v}(b)| - 1$ when b ranges over V(T).

We give an example of tree decomposition in Figure 2:

• In Figure 2a, we give the "full" representation of the decomposition: we draw T, and inside each bag b of T we represent a copy of G. Nodes of G belonging to b are highlighted, while the others are dimmed. Sometimes, we will only write the name of the nodes contained in the bag, instead of drawing the graph.

⁴Theorem 3 talks about query containment of CQs, which is in fact equivalent to the evaluation problem for CQs. Moreover, the theorem deals with "query width", but this parameter is equivalent up to a multiplicative constant to the tree-width [CR00, Lemma 2] assuming that the database signature arity is fixed.

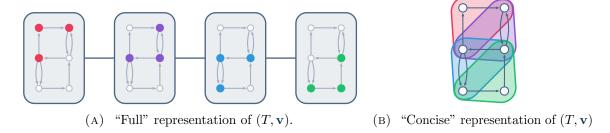


FIGURE 2. Two different representations of the same tree decomposition (T, \mathbf{v}) of a multigraph G with six vertices. The underlying tree is a path with four nodes and each bag contains 3 vertices—hence the decomposition has width 2.

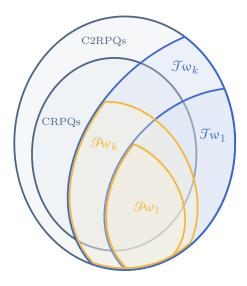


FIGURE 3. Clickable taxonomy of syntactic classes studied in this paper.

• In Figure 2b, we give a "concise" representation: we draw over G a coloured shape for each bag of T. This representation is ambiguous—the structure of T is not made explicit—and will only be used when no ambiguity can arise.

The tree-width of G is the minimum of the width of all tree decompositions of G. The tree-width of a C2RPQ is the tree-width of its underlying multigraph. We denote by $\mathcal{T}\omega_k$ (resp. $1\mathcal{T}\omega_k$) the set of all C2RPQs (resp. CRPQs) of tree-width at most k. The tree-width of a UC2RPQ is simply the maximum of the tree-width of its C2RPQs. A path decomposition is a tree decomposition (T, \mathbf{v}) in which T is a path. The path-width of γ is the minimum of the width among all path decompositions of γ . The path-width of a C2RPQ and UC2RPQ are defined analogously. We denote by $\mathcal{P}\omega_k$ (resp. $1\mathcal{P}\omega_k$) the set of all C2RPQs (resp. CRPQs) of path-width at most k. The relationship between these classes is depicted in Figure 3: note that $1\mathcal{T}\omega_k$ and $1\mathcal{P}\omega_k$ are not explicitly drawn, but correspond to the intersection of $\mathcal{T}\omega_k$ (resp. $\mathcal{P}\omega_k$) with the class of CRPQs.

Similar statements of the following proposition can be considered Folklore (see *e.g.* [RBV17, Theorem IV.3]); however, our inability to find a proof for it with sharp bounds invites us to include a proof.

Proposition 1.1 (Proof in Appendix A). For each $k \ge 1$, the evaluation problem for UC2RPQs of tree-width at most k can be solved in time $\Theta(\|\Gamma\| \cdot |G|^{k+1} \cdot \log |G|)$ on a Turing machine, or $\Theta(\|\Gamma\| \cdot |G|^{k+1})$ under a RAM model, where Γ and G are the input UC2RPQ and graph database, respectively.

In practice, graph databases tend to be huge and often changing, while queries are in comparison very small. This motivates the following question, given some natural $k \ge 1$:

Given a UC2RPQ Γ , is it equivalent to a UC2RPQ Γ' of tree-width at most k? That is, does it have *semantic tree-width* at most k?

This problem is called the *semantic tree-width k problem*. Should it be decidable in a constructive way—that is, decidable, and if the answer is positive, we can compute a witnessing Γ' from Γ —, then one could, once and for all, compute Γ' from Γ and, whenever one wants to evaluate Γ on a database, evaluate Γ' instead.

We will also study the restriction of these notions to one-way queries: a UCRPQ has one-way semantic tree-width at most k if it is equivalent to a UCRPQ of tree-width at most k. The one-way semantic tree-width k problem is the problem of, given a UCRPQ Γ , whether it has one-way semantic tree-width at most k.

Example 1.2. Consider the following CRPQs, where $\bar{x} = (x_0, x_1, y, z)$:

$$\gamma(\bar{x}) \stackrel{c}{=} \begin{matrix} x_0 & \xrightarrow{c} & x_1 \\ y \\ a(bb)^+ & \downarrow b^+ & ab(bb)^* \end{matrix} \qquad \delta(\bar{x}) \stackrel{c}{=} \begin{matrix} x_0 & \xrightarrow{c} & x_1 \\ y \\ z \end{matrix} \qquad \delta'(\bar{x}) \stackrel{c}{=} \begin{matrix} x_0 & \xrightarrow{c} & x_1 \\ y \\ y \end{matrix} \qquad \delta'(\bar{x}) \stackrel{c}{=} \begin{matrix} x_0 & \xrightarrow{c} & x_1 \\ y \\ z \end{matrix} \qquad \delta(bb)^+ \downarrow \begin{matrix} ab(bb)^* \\ z \end{matrix} \qquad bb(bb)^* \qquad bb(bb)^$$

The underlying graph of $\gamma(\bar{x})$ being the directed 4-clique, $\gamma(\bar{x})$ has tree-width 3. We claim that $\gamma(\bar{x})$ is equivalent to the UCRPQ $\delta(\bar{x}) \vee \delta'(\bar{x})$, and hence has one-way semantic tree-width at most 2.

Indeed, given a graph database satisfying $\gamma(\bar{x})$ via some mapping μ , it suffices to make a case disjunction on whether the number of b-labelled atoms in the path from $\mu(y)$ to $\mu(z)$ is even or odd. In the first case, the atom $x_0 \xrightarrow{a(bb)^+} z$ becomes redundant since we can deduce the existence of such a path from the conjunction $x \xrightarrow{a} y \xrightarrow{(bb)^+} z$, and hence the database satisfies $\delta(\bar{x})$ via μ . Symmetrically, in the second case, the atom $x_1 \xrightarrow{b(bb)^*} z$ becomes redundant, and the database satisfies $\delta'(\bar{x})$ via μ . Thus, $\gamma(\bar{x})$ is contained, and hence equivalent (the other containment being trivial), to the UCRPQ $\delta(\bar{x}) \vee \delta'(\bar{x})$ of tree-width 2.

1.2. **Related Work.** On the class conjunctive queries, the semantic tree-width k problem becomes the coNP-complete problem of finding out whether the retraction of a query has tree-width at most k. In fact, CQs enjoy the effective existence of unique minimal queries [CM77, Theorem 12], which happen to also minimize the tree-width. For CRPQs and UC2RPQs, the question is far more challenging, and it has only been solved for the case

⁵In this graphical representation, we interpret a labelled graph as the CRPQ defined as the conjunction of the atoms induced by the labelled edges of the graph. For instance, $\gamma(\bar{x})$ is a conjunction of six atoms.

k=1 by Barceló, Romero, and Vardi [BRV16, Theorem 6.1]; the case k>1 was left widely open [BRV16, §7].

Furthermore, classes of CQs of bounded semantic tree-width precisely characterize tractable (and FPT) evaluation problem [Gro07, Theorem 1.1]. This result is on bounded-arity schemas, which was later generalized [CGLP20, Theorem 1] for characterizing FPT evaluation on arbitrary schemas—by replacing semantic tree-width with semantic "submodular width" [Mar13].

The problem of computing maximal under-approximations of CQs of a given tree-width has been explored in [BLR14]. A maximal under-approximations of tree-width at most k of a CQ γ consists of a CQ δ_k of tree-width at most k, which under-approximates it, i.e. δ_k is contained in γ , and which is maximal, in the sense that for every CQ δ' , if δ' has tree-width at most k and is contained in γ , then δ' is contained in δ_k . Maximal under-approximations of a given tree-width for CQs always exist [BLR14] and thus, a CQ is semantically equivalent to a CQ of tree-width at most k if, and only if, it is equivalent to its maximal under-approximation of tree-width at most k. Our solution to decide the semantic tree-width k problem for UC2RPQs is based on this idea.

While maximal under-approximations always exist for CQs, this is not the case for the dual notion of "minimal over-approximations". The problem of when these exist is still unknown to be decidable, aside for some the special cases of acyclic CQs and Boolean CQs over binary schemas [BRZ20].

1.3. Contributions. Here we solve both the semantic tree-width k problem and one-way semantic tree-width k problem for every k with one unifying approach.

Theorem 1.3. For each $k \ge 1$, the semantic tree-width k problem and the one-way semantic tree-width k problem are decidable. Moreover, these problems are in 2ExpSpace and are 2ExpSpace and 2ExpSpace are in fact 2ExpSpace.

In Section 3 (Lemma 3.10), we prove the upper bound for $k \ge 2$, by relying on the so-called "Key Lemma", which is our main technical result, and is proven in Sections 4 and 5. The upper bound for the case k = 1—which was already proven in [BRV16] for the (two-way) semantic tree-width 1 problem—is shown in Section 7 (Corollary 7.8). The lower bound is shown in Section 9 (Lemma 9.1).

The Key Lemma (Lemma 3.8) essentially states that every UC2RPQ has a computable "maximal under approximation" by a UC2RPQ of tree-width k and that this approximation is well-behaved with respect to the class of languages used to label the queries under some mild assumptions on it (being "closed under sublanguages"). Let us first explain this assumption before formalizing the statement above (stated as Corollary 3.9).

For a class \mathcal{L} of languages, let $\mathrm{UC2RPQ}(\mathcal{L})$ denote the class of all $\mathrm{UC2RPQS}$ whose atoms are all labelled by languages from \mathcal{L} . For an NFA \mathcal{A} and two states q, q' thereof, we denote by $\mathcal{A}[q,q']$ the *sublanguage* of \mathcal{A} recognized when considering $\{q\}$ as the set of initial states and $\{q'\}$ as the set of final states. We say that \mathcal{L} is *closed under sublanguages* if (i) it contains every language of the form $\{a\}$, where $a \in \mathbb{A}$ is any (positive) letter such that either a or a^- occur in a word of a language of \mathcal{L} , and (ii) for every language $L \in \mathcal{L}$ there exists an NFA \mathcal{A}_L accepting L such that every sublanguage $\mathcal{A}_L[q,q']$ distinct from \emptyset and $\{\varepsilon\}$ belongs to \mathcal{L} .

To the best of our knowledge, all classes of regular expressions that have been considered in the realm of regular path queries (see, e.g., [FGK⁺20, §1]) are closed under sublanguages.

In particular, this is the case for the class $\{\{a_1 + \ldots + a_n\} \mid a_1, \ldots, a_n \in \mathbb{A}\} \cup \{a^* \mid a \in \mathbb{A}\}$, which will be our focus of study in Section 6. Moreover, even if some class \mathcal{L} is not closed under sublanguages, such as $\{(aa)^*\}$, then it is contained in a minimal class closed under sublanguages— $\{a, a(aa)^*, (aa)^*\}$ in this example.

We can now state the main implication of the Key Lemma (whose formal statement requires some extra definitions).

Corollary 3.9 (Existence of the maximal under-approximation). For each $k \geq 2$, for each class \mathcal{L} closed under sublanguages, and for each query $\Gamma \in \text{UC2RPQ}(\mathcal{L})$, there exists $\Gamma' \in \text{UC2RPQ}(\mathcal{L})$ of tree-width at most k such that $\Gamma' \subseteq \Gamma$, and for every $\Delta \in \text{UC2RPQ}$, if Δ has tree-width at most k and $\Delta \subseteq \Gamma$, then $\Delta \subseteq \Gamma'$. Moreover, Γ' is computable from Γ in ExpSpace.

As a consequence of Corollary 3.9 and Proposition 1.1, we have that queries of bounded semantic tree-width have tractable evaluation.

Corollary 3.16 (FPT evaluation for bounded semantic tree-width). For each $k \ge 1$, the evaluation problem for C2RPQs of semantic tree-width at most k is fixed-parameter tractable—FPT—when parametrized in the size of the query. More precisely on input $\langle \Gamma, G \rangle$, the algorithm runs in time $\Theta(f(\|\Gamma\|) \cdot |G|^{k+1} \cdot \log |G|)$ on a Turing machine, where f is a doubly-exponential function—or $\Theta(f(\|\Gamma\|) \cdot |G|^{k+1})$ under a RAM model.

Note that [FGM24, Theorem 22] shows that the statement above can be improved to have a single-exponential function f.

Moreover, we also show that for any class \mathcal{L} of regular languages closed under sublanguages, if $\Gamma \in \text{UC2RPQ}(\mathcal{L})$ has semantic tree-width k > 1, then Γ is equivalent to a UC2RPQ(\mathcal{L}) of tree-width at most k. Analogous characterizations hold for k = 1 and/or path-width, see Corollaries 8.8 and 7.9.

Theorem 3.13. Assume that \mathcal{L} is closed under sublanguages. For any k > 1 and any query $\Gamma \in \text{UC2RPQ}(\mathcal{L})$, the following are equivalent:

- (1) Γ is equivalent to an infinitary union of conjunctive queries of tree-width at most k;
- (2) Γ has semantic tree-width at most k;
- (3) Γ is equivalent to a UC2RPQ(\mathcal{L}) of tree-width at most k.

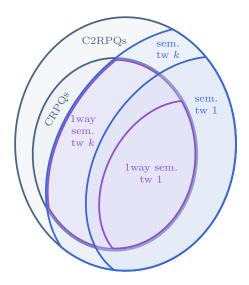
The implications $(3) \Rightarrow (2) \Rightarrow (1)$ immediately follow from the definition of the semantic tree-width. On the other hand, the implications $(1) \Rightarrow (2)$ and $(2) \Rightarrow (3)$ are surprising, since they are both trivially false when k = 1. We defer the proof of this last claim to Remark 3.14 as we first need a few tools to manipulate CRPQs.

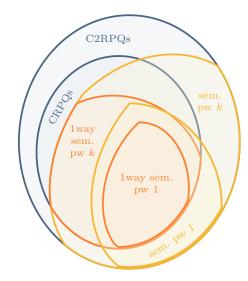
The previous theorem, together with the high complexity of semantic tree-width k problem, motivates us to focus on the case of CRPQs using some simple regular expressions (SRE) in Section 6, where we show that the complexity of this problem is much lower.

Theorem 6.1. For $k \ge 2$, the semantic tree-width k problem for UCRPQ(SRE) is in Π_2^p .

We then study the problem of k=1: at first glance, our proof for $k \ge 2$ of Theorem 1.3 does not capture this case, for a technical—yet crucial—reason. In Section 7, we explain how to adapt our proof to capture it: and show the decidability the semantic tree-width 1 problem—which was already studied by Barceló, Romero and Vardi [BRV16]—and of the one-way semantic tree-width 1 problem.

Building on the same idea, we show in Section 8 that our results extend to path-width.





- (A) Semantic classes of C2RPQs related to tree-width.
- (B) Semantic classes of C2RPQs related to path-width.

FIGURE 4. Clickable taxonomy of semantic classes studied in this paper, where $k \ge 2$.

Theorem 8.7. For each $k \ge 1$, the semantic path-width k problems are decidable. Moreover, they lie in $2\mathsf{ExpSpace}$ and are $\mathsf{ExpSpace}$ -hard. Moreover, if k=1, these problems are in fact $\mathsf{ExpSpace}$ -complete.

In turn, this leads to an evaluation algorithm with a remarkably low complexity.

Theorem 8.9. For each $k \ge 1$, the evaluation problem, restricted to UC2RPQs of semantic path-width at most k is in paraNL when parametrized in the size of the query. More precisely, the problem, on input $\langle \Gamma, G \rangle$, can be solved in non-deterministic space $f(|\Gamma|) + \log(|G|)$, where f is a single exponential function.

Interestingly, the proof for tree-width 1 and path-width k ($k \ge 1$) can be derived from the proof from tree-width $k \ge 2$ but necessitates an additional technical trick which yields different closure properties (or lack thereof). We show that a UCRPQ has semantic tree-width at most k if, and only if, it has one-way semantic tree-width at most k whenever $k \ge 2$ (Corollary 3.15). In other words, if the original query does not use two-way navigation, then considering UC2RPQs does not help to further minimize the tree-width. Interestingly, this is false for k = 1 (cf. Remark 3.14, also [BRV16, Proposition 6.4]) and for path-width, no matter the value of $k \ge 1$ (see Remark 8.2). Overall, this leads to the landscape depicted in Figure 4.

Finally, we conclude in Section 10. We provide a partial characterization à la Grohe of classes of UC2RPQs which admit a tractable evaluation in Section 10.2.

Theorem 10.5. Assuming W[1] \neq FPT, for any recursively enumerable class C of finitely-redundant Boolean UC2RPQs, the evaluation problem for C is FPT if, and only if, C has bounded semantic tree-width.

We also discuss open questions, ranging from complexity questions (Section 10.1) to extensions of our results to bigger classes or larger settings (Sections 10.3 and 10.4).

1.4. Conference Paper. The current article is based on the conference paper [FM23]. The main results for tree-width k > 1 are essentially the same—though with improved explanations and figures, and we fixed some minor bugs in the proof of the Key Lemma. Here we also show how to extend our techniques to tackle the semantic tree-width 1 problem (Section 7) and we introduce and study the semantic path-width k problems (Section 8). Our very partial lift of Grohe's characterization of FPT classes of queries (Theorem 10.5) is also new.

2. Preliminaries

Before attacking the statement of our Key Lemma in Section 3, we first give a few elementary definitions on C2RPQs in this section. We write \mathbb{N} to denote $\{0,1,\dots\}$ and [i,j] to denote $\{n\in\mathbb{N}:i\leqslant n\leqslant j\}$. A homomorphism f from a C2RPQ $\gamma(x_1,\dots,x_m)$ to a C2RPQ $\gamma'(y_1,\dots,y_m)$ is a mapping from $vars(\gamma)$ to $vars(\gamma')$ such that $f(x)\stackrel{L}{\longrightarrow} f(y)$ is an atom of γ' for every atom $x\stackrel{L}{\longrightarrow} y$ of γ , and further $f(x_i)=y_i$ for every i. Such a homomorphism f is strong onto if for every atom $x'\stackrel{L}{\longrightarrow} y'$ of γ' there is an atom $x\stackrel{L}{\longrightarrow} y$ of γ such that f(x)=x' and f(y)=y'. An example of homomorphism is provided in Figure 5b. We write $\gamma \stackrel{hom}{\longrightarrow} \gamma'$ if there is a homomorphism from γ to γ' , and $\gamma \stackrel{hom}{\longrightarrow} \gamma'$ if there is a strong onto homomorphism. In the latter case, we say that γ' is a homomorphic image of γ . It is easy to see that if $\gamma \stackrel{hom}{\longrightarrow} \gamma'$ then $\gamma' \subseteq \gamma$, and in the case where γ, γ' are CQs this is an "if and only if" [CM77, Lemma 13].

Some intuitions on maximal under-approximations. Given a conjunctive query γ , the union of all conjunctive queries that are contained in γ is semantically equivalent to the union $\bigvee \{\gamma' \mid \gamma \xrightarrow{hom} \gamma'\}$. Naturally, this statement borders on the trivial since γ' belongs to this union. It becomes interesting when we add a restriction: given a class C of CQs (to which γ may not belong) closed under subqueries, then $\Gamma' = \bigvee \{\gamma' \in C \mid \gamma \xrightarrow{hom} \gamma'\}$ is the maximal under-approximations of γ by finite unions of conjunctive queries of C, in the following sense:

- i. (finite) Γ' is a finite union of CQs of C,
- ii. (under-approximation) $\Gamma' \subseteq \gamma$, and
- iii. (maximality) for any finite union Δ of CQs of C, if $\Delta \subseteq \gamma$, then $\Delta \subseteq \Gamma'$.

Proof. Only the last point is non-trivial, and follows from the fact that if $\Delta \subseteq \gamma$, then for each $\delta \in \Delta$, $\delta \subseteq \gamma$, so there is a homomorphism $f \colon \gamma \to \delta$. The image δ' of f is a subquery of δ , and \mathcal{C} is closed under subqueries, so it belongs to \mathcal{C} , and hence to Γ' . Since there is a trivial homomorphism from δ' to δ , we moreover have that $\delta \subseteq \delta'$. Hence, for each CQ $\delta \in \Delta$, there is a CQ $\delta' \in \Gamma'$ such that $\delta \subseteq \delta'$, and hence $\Delta \subseteq \Gamma'$.

As a consequence, we deduce that for each $k \ge 1$, the maximal under-approximation of a CQ by a finite union of CQs of tree-width at most k is computable, and hence we can effectively decide if some CQ is equivalent to a query of tree-width at most k by testing the equivalence with this maximal under-approximation. For more details on approximations of CQs, see [BLR14]. Note that interestingly, changing Γ' from $\bigvee \{\gamma' \in C \mid \gamma \xrightarrow{hom} \gamma'\}$ to

 $\bigvee \{\gamma' \in \mathcal{C} \mid \gamma' \subseteq \gamma\}$ preserves both under-approximation and maximality, but Γ' is now an infinite union of CQs of \mathcal{C} .

Unfortunately, these results cannot be straightforwardly extended to conjunctive regular path queries since the previous proof implicitly relied on two points:

- (1) the equivalence between the containment $\gamma' \subseteq \gamma$ and the existence of a homomorphism $\gamma \xrightarrow{hom} \gamma'$, and
- (2) the possibility to restrict γ' to its image $\gamma \xrightarrow{hom} \gamma'$ while obtaining a semantically bigger query.

These two crucial ingredients is what allows us to build a finite set Γ' from γ . For CRPQs, the second point still holds, but not the first one. For instance, the CQ $\gamma(x,y)=x\overset{a}{\to}z\overset{b}{\to}y$ is contained in (in fact equivalent to) the CRPQ $\gamma'(x,y)=x\overset{ab}{\to}y$, but there is no homomorphism from $\gamma'(x,y)$ to $\gamma(x,y)$. Our main result shows that to find maximal under-approximations of C2RPQs, it suffices to take homomorphic images of so-called "refinements" of γ , instead of homomorphic images of γ itself. The next paragraphs are devoted to introducing refinements and tools related to them.

Equality Atoms. C2RPQs with equality atoms are queries of the form $\gamma(\bar{x}) = \delta \wedge I$, where δ is a C2RPQ (without equality atoms) and I is a conjunction of equality atoms of the form x=y. Again, we denote by $vars(\gamma)$ the set of variables appearing in the (equality and non-equality) atoms of γ . We define the binary relation $=_{\gamma}$ over $vars(\gamma)$ to be the reflexive-symmetric-transitive closure of the binary relation $\{(x,y) \mid x=y \text{ is an equality atom in } \gamma\}$. In other words, we have $x=_{\gamma}y$ if the equality x=y is forced by the equality atoms of γ . Note that every C2RPQ with equality atoms $\gamma(\bar{x}) = \delta \wedge I$ is equivalent to a C2RPQ without equality atoms γ^{\approx} , which is obtained from γ by collapsing each equivalence class of the relation $=_{\gamma}$ into a single variable. This transformation gives us a canonical renaming from $vars(\gamma)$ to $vars(\gamma^{\approx})$. For instance, $\gamma(x,y) = x \xrightarrow{K} y \wedge y \xrightarrow{L} z \wedge x = y$ collapses to $\gamma^{\approx}(x,x) = x \xrightarrow{K} x \wedge x \xrightarrow{L} z$.

Refinements. An atom m-refinement of a C2RPQ atom $\gamma(x,y) = x \xrightarrow{L} y$ where L is given by the NFA \mathcal{A}_L is any C2RPQ of the form

$$\rho(x,y) = x \xrightarrow{L_1} t_1 \xrightarrow{L_2} \dots \xrightarrow{L_{n-1}} t_{n-1} \xrightarrow{L_n} y$$
 (2.1)

where $1 \leq n \leq m$, t_1, \ldots, t_{n-1} are fresh (existentially quantified) variables, and L_1, \ldots, L_n are such that there exists a sequence (q_0, \ldots, q_n) of states of \mathcal{A}_L such that q_0 is initial, q_n is final, and for each i, L_i is either of the form

- (i) $\mathcal{A}_L[q_i, q_{i+1}],$
- (ii) $\{a\}$ if the letter $a \in \mathbb{A}$ belongs to $\mathcal{A}_L[q_i, q_{i+1}]$, or
- (iii) $\{a^-\}$ if $a^- \in \mathbb{A}^-$ belongs to $\mathcal{A}[q_i, q_{i+1}]$.

Additionally, if $\varepsilon \in L$, the equality atom "x = y" is also an atom m-refinement. Thus, an atom m-refinement can be either of the form (2.1) or "x = y". By convention, $t \xrightarrow{a^-} t'$ is a shorthand for $t' \xrightarrow{a} t$. As a consequence, the underlying graph of an atom m-refinement of the form (2.1) is not necessarily a directed path. By definition, note that $L_1 \cdots L_n \subseteq L$ and hence $\rho \subseteq \gamma$ for any atom m-refinement ρ of γ . An atom refinement is an atom m-refinement for some m. An example is provided in Figure 5a.

Definition 2.1. Given an atom refinement $\rho = x \xrightarrow{L_1} t_1 \xrightarrow{L_2} \dots \xrightarrow{L_{n-1}} t_{n-1} \xrightarrow{L_n} y$ of $\gamma = x \xrightarrow{L} y$ as in (2.1), define a *condensation* of ρ between t_i and t_j , where $0 \le i, j \le n$ and

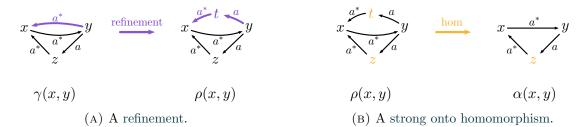


FIGURE 5. Refinements and homomorphisms of C2RPQs.

j > i + 1, as any C2RPQ of the form:

$$\rho' = x \xrightarrow{L_1} t_1 \xrightarrow{L_2} \dots \xrightarrow{L_i} t_i \xrightarrow{K} t_j \xrightarrow{L_{j+1}} \dots \xrightarrow{L_{n-1}} t_{n-1} \xrightarrow{L_n} y$$

such that $K = \mathcal{A}[q_i, q_i]$.

Fact 2.2. Every condensation ρ' of ρ is a refinement of γ , and $\rho \subseteq \rho' \subseteq \gamma$.

Informally, we will abuse the notation and write $[L_i \cdots L_j]$ to denote the language K—even if this language does not only depend on $L_i \cdots L_j$.

Example 2.3. Let $\gamma(x,y) = x \xrightarrow{(aa^-)^*} y$ be a C2RPQ atom, where $(aa^-)^*$ is implicitly represented by its minimal automaton. Then $\rho(x,y)$ is a refinement of refinement length seven of $\gamma(x,y)$ and $\rho'(x,y)$ is a condensation of $\rho(x,y)$, where:

$$\rho(x,y) = x \xrightarrow{a} t_1 \xrightarrow{(a^-a)^*} t_2 \xrightarrow{(a^-a)^*} t_3 \xleftarrow{a} t_4 \xrightarrow{(aa^-)^*} t_5 \xrightarrow{(aa^-)^*a} t_6 \xleftarrow{a} y,$$

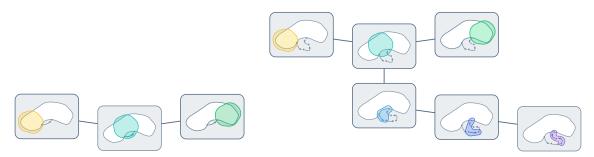
$$\rho'(x,y) = x \xrightarrow{a} t_1 \xrightarrow{(a^-a)^*} t_2 \xrightarrow{(a^-a)^*} t_3 \xleftarrow{a} t_4 \xrightarrow{(aa^-)^*} y.$$

On the other hand, $\rho''(x,y) = x \xrightarrow{a} t_1 \xleftarrow{a} y$ is not a condensation of $\rho(x,y)$.

Given a natural number m, an m-refinement of a C2RPQ $\gamma(\bar{x}) = \bigwedge_i x_i \xrightarrow{L_i} y_i$ is any query resulting from: 1) replacing every atom by one of its m-refinements, and 2) should some m-refinements have equality atoms, collapsing the variables. A refinement is an m-refinement for some m. Note that any atom m-refinements is, by definition, also an atom m'-refinements when $m \leq m'$: as a consequence, in the refinement of a C2RPQ the atom refinements need not have the same length. For instance, both $\rho(x,x) = x \xrightarrow{c} x$ and $\rho'(x,y) = x \xrightarrow{a} t_1 \xrightarrow{a} y \xrightarrow{c} y$ are refinements of $\gamma(x,y) = x \xrightarrow{a^*} y \xrightarrow{c} x$.

For a given C2RPQ γ , let $\text{Ref}^{\leqslant m}(\gamma)$ be the set of all m-refinements of γ , and $\text{Ref}(\gamma)$ be the set of all its refinements. Given a refinement $\rho(\bar{x})$ of $\gamma(\bar{x})$, its refinement length is the least natural number m such that $\rho(\bar{x}) \in \text{Ref}^{\leqslant m}(\gamma)$. Note that if the automaton representing a language L has more than one final state, for instance the minimal automaton for $L = a^+ + b^+$, then $x \xrightarrow{L} y$ is not a refinement of itself. However, it will always be equivalent to a union of refinements: in this example, $x \xrightarrow{a^+ + b^+} y$ is equivalent to the union of $x \xrightarrow{a^+} y$ and $x \xrightarrow{b^+} y$, which are both refinements of the original C2RPQ.

Expansions. Remember that a C2RPQ whose languages are of the form $\{a\}$ or $\{a^-\}$ for $a \in \mathbb{A}$ is in effect a CQ. The *expansions* of a C2RPQ γ is the set $\text{Exp}(\gamma)$ of all CQs which are refinements of γ . In other words, an expansion of γ is any CQ obtained from γ by replacing each atom $x \xrightarrow{L} y$ by a path $x \xrightarrow{w} y$ for some word $w \in L$. For instance, $\xi(x,y) = x \xrightarrow{a} t_1 \xleftarrow{a} t_2 \xrightarrow{a} t_3 \xleftarrow{a} y$ is an expansion of $\rho(x,y) = x \xrightarrow{(aa^-)^*} y$.



decomposition of width k.

(A) A multigraph together with a tree (B) A refinement of the multigraph of Figure 6a together with a tree decomposition of width $\max(k, 2)$.

FIGURE 6. Refinements and expansions preserve tree-width at most $k \ge 2$.

Any C2RPQ is equivalent to the infinitary union of its expansions. In light of this, the semantics for UC2RPQ can be rephrased as follows. Given a UC2RPQ $\Gamma(\bar{x})$ and a graph database G, the evaluation of $\Gamma(\bar{x})$ over G, denoted by $\Gamma(G)$, is the set of tuples \bar{v} of nodes for which there is $\xi \in \text{Exp}(\Gamma)$ such that there is a homomorphism $\xi \xrightarrow{hom} G$ that sends \bar{x} onto \bar{v} . Similarly, containment of UC2RPQs can also be characterized in terms of expansions.

Proposition 2.4 (Folklore, see e.g. [FLS98, Proposition 3.2] or [CDLV00, Theorem 2]). Let Γ_1 and Γ_2 be UC2RPQs. Then the following are equivalent

- $\Gamma_1 \subseteq \Gamma_2$;
- for every $\xi_1 \in \text{Exp}(\Gamma_1)$, $\xi_1 \subseteq \Gamma_2$;
- for every $\xi_1 \in \operatorname{Exp}(\Gamma_1)$ there is $\xi_2 \in \operatorname{Exp}(\Gamma_2)$ such that $\xi_2 \xrightarrow{hom} \xi_1$.

Note that since an expansion of γ is also a refinement of γ , it also holds that γ is semantically equivalent to the infinitary union of its refinements.

Our approach to proving Theorems 1.3 and 3.13 and the Key Lemma heavily rely on refinements. One crucial property that these objects satisfy is that they preserve tree-width k, unless k=1, as illustrated in Figure 6.

Fact 2.5. Let $k \ge 2$ and let γ be a C2RPQ of tree-width at most k. Then any refinement of γ has tree-width at most k.

Proof. The underlying graph of a refinement of γ is obtained from the underlying graph of γ by either contracting some edges (when dealing with equality atoms), or by replacing a single edge by a path of edges (where the non-extremal nodes are new nodes).

This first operation preserves tree-width at most k (even if k=1), see e.g. [Bod98, Lemma 16. The second operation preserves tree-width at most k, assuming k > 1: if a graph G' is obtained from a graph G by replacing an edge $x_0 \to x_n$ by a path $x_0 \to x_1 \to \cdots \to x_n$, then from a tree decomposition of G it suffices to pick a bag containing both x_0 and x_n , and add a branch to the tree, rooted at this bag, and containing bags with nodes

$$\{x_0, x_1, x_n\}, \{x_1, x_2, x_n\}, \dots, \{x_i, x_{i+1}, x_n\}, \dots, \{x_{n-2}, x_{n-1}, x_n\},$$

as depicted in Figure 6. All bags contain exactly three nodes, so we obtain tree decomposition of G' whose width is the maximum between 2 and the width of the original tree decomposition of G.

For k=1, the property fails: for instance the CRPQ $\gamma(x)=x\xrightarrow{a^*}x$ has tree-width at most 1 (in fact it has tree-width 0), but its refinement $\rho(x)=x\xrightarrow{a^*}t_1\xrightarrow{a^*}t_2\xrightarrow{a^*}x$ has tree-width 2.

Fine tree decompositions. For technical reasons—the proof of Lemma 5.4—, we will use a restrictive class of tree decompositions which we call "fine" 6 . A *fine tree decomposition* is a tree decomposition (T, \mathbf{v}) in which:

In the context of a fine tree decomposition of width k, a full bag is any bag of size k+1.

A C2RPQ has tree-width k if and only if it has a fine tree decomposition of width at most k. Indeed, from a tree decomposition, it suffices to:

- (1) first merge every consecutive pair of bags that contain exactly the same variables;
- (2) between every pair of bags that does not satisfy (2.2), add a bag whose set of vertices correspond to the intersection of the two adjacent bags.

3. Maximal Under-Approximations

In this section, we state our key technical result, Lemma 3.8, which we will refer to as the "Key Lemma". Essentially, we follow the same structure as Theorem 3.13: given a C2RPQ γ and a natural number k > 1, we start by considering its maximal under-approximation by infinitary unions of conjunctive queries of tree-width k (Definition 3.1), and then show that this query can in fact be expressed as a UC2RPQ of tree-width k whose atoms contain sublanguages of those in γ (Key Lemma 3.8).

For the first definitions of this section, let us fix any class C of C2RPQs—we will later apply these results to the class $\mathcal{T}\omega_k$ of C2RPQs of tree-width at most k.

Definition 3.1 (Maximal under-approximation). Let γ be a C2RPQ. The maximal under-approximation of γ by infinitary unions of C-queries is $App_{\mathcal{C}}(\gamma) = \{\alpha \in \mathcal{C} \mid \alpha \subseteq \gamma\}$.

For intuition, we refer the reader back to paragraph "Some intuitions on maximal under-approximations" at the beginning of Section 2.

Remark 3.2. Observe that $App_{\mathcal{C}}(\gamma)$ is an infinitary union of \mathcal{C} -queries, that $App_{\mathcal{C}}(\gamma) \subseteq \gamma$, and that for every infinitary union of \mathcal{C} -queries Δ , if $\Delta \subseteq \gamma$, then $\Delta \subseteq App_{\mathcal{C}}(\gamma)$ (*i.e.*, it is the unique maximal under-approximation up to semantical equivalence). Similarly, the maximal under-approximation of a UC2RPQ is simply the union of the maximal under-approximations of the C2RPQs thereof.

Unfortunately, the fact that a query α is part of this union, namely $\alpha \in \operatorname{App}_{\mathcal{C}}(\gamma)$, does not yield any useful information on the *shape* of α —we merely know that $\alpha \subseteq \gamma$. We thus introduce another infinitary union of \mathcal{C} -queries of a restricted shape, namely $\operatorname{App}_{\mathcal{C}}^*(\gamma) \subseteq \operatorname{App}_{\mathcal{C}}(\gamma)$, in which queries $\alpha \in \operatorname{App}_{\mathcal{C}}^*(\gamma)$ come together with a witness of their containment in γ .

 $^{^6}$ This is similar—but orthogonal—to the classical notion of "nice tree decomposition", see *e.g.* [Klo94, Definition 13.1.4, page 149].

Definition 3.3. The maximal under-approximation of γ by infinitary unions of homomorphically-smaller C-queries is

$$\operatorname{App}_{\mathcal{C}}^{\star}(\gamma) = \{ \alpha \in \mathcal{C} \mid \exists \rho \in \operatorname{Ref}(\gamma), \exists f : \rho \xrightarrow{hom} \alpha \}.$$
 (3.1)

For a basic example of approximation (with no constraint on C), we refer the reader to Figure 5. The resulting query $\alpha(x,y)$ is the homomorphic image of a refinement of $\gamma(x,y)$. Hence, $\alpha(x,y) \in \mathrm{App}_{\mathcal{C}}^{\star}(\gamma)$ if C is, for instance, the class of all C2RPQs—or more generally, if C contains $\alpha(x,y)$.

Example 3.4 (Example 1.2, cont'd). Both $\delta(\bar{x})$ and $\delta'(\bar{x})$ are semantically equivalent to queries in $\text{App}_{T\omega_2}^{\star}(\gamma(\bar{x}))$. Indeed, starting from $\gamma(\bar{x})$, we can refine

$$x_0 \xrightarrow{a(bb)^+} z$$
 into $x_1 \xrightarrow{a} t \xrightarrow{(bb)^+} z$.

Denote by $\rho(\bar{x})$ the query obtained:

$$\rho(\bar{x}) \stackrel{c}{=} t \stackrel{x_0}{\underset{(bb)^+}{\longrightarrow}} x_1 \qquad x_0 \stackrel{c}{\underset{\bar{x}_0}{\longrightarrow}} x_0 \qquad x_0 \stackrel{c}{\underset{\bar{x}_0}{\longrightarrow}} x_0$$

Then merge variables t and y: this new query $\delta'_{\rm app}(\bar{x})$ is equivalent to $\delta'(\bar{x})$. Moreover, since $\delta'_{\rm app}(\bar{x})$ has tree-width at most 2 and was obtained as a homomorphic image of a refinement of $\gamma(\bar{x})$, we have that $\delta'_{\rm app}(\bar{x}) \in {\rm App}^{\star}_{\mathcal{T}_{\omega_2}}(\gamma(\bar{x}))$. A similar argument applies to δ , by refining the atom between x_1 and z instead.

Clearly, $\operatorname{App}_{\mathcal{C}}^{\star}(\gamma)$ —whose queries are informally called *approximations*—is included, and thus semantically contained, in $\operatorname{App}_{\mathcal{C}}(\gamma)$, since $\rho \subseteq \gamma$ and $\alpha \subseteq \rho$ in (3.1). In fact, under some assumptions on \mathcal{C} , the converse containment also holds.

Observation 3.5. If C is closed under expansions and subqueries, then for any C2RPQ γ , we have $App_C(\gamma) \equiv App_C^*(\gamma)$.

Proof. Since $\operatorname{App}_{\mathcal{C}}(\gamma) \supseteq \operatorname{App}_{\mathcal{C}}^{\star}(\gamma)$, it suffices to show that $\operatorname{App}_{\mathcal{C}}(\gamma) \subseteq \operatorname{App}_{\mathcal{C}}^{\star}(\gamma)$. Pick $\alpha \in \operatorname{App}_{\mathcal{C}}(\gamma)$. Let ξ be an expansion of α . Since $\alpha \subseteq \gamma$, there exists by Proposition 2.4 an expansion ξ_{γ} of γ such that $\xi_{\gamma} \xrightarrow{hom} \xi$. Consider the restriction ξ' of ξ to its homomorphic image. Since $\alpha \in \mathcal{C}$ and \mathcal{C} is closed both under expansions and subqueries, $\xi' \in \mathcal{C}$. Since moreover, by construction, ξ' is the (strong onto) homomorphic image of an expansion (hence refinement) of γ , then $\xi' \in \operatorname{App}_{\mathcal{C}}^{\star}(\gamma)$. Hence, we have shown that for every expansion of $\operatorname{App}_{\mathcal{C}}(\gamma)$, there is an expansion of $\operatorname{App}_{\mathcal{C}}(\gamma)$ with a strong onto homomorphism from the latter to the former, which concludes the proof by Proposition 2.4.

Note that in the definition of $\operatorname{App}_{\mathcal{C}}^{\star}(\gamma)$ we work with strong onto homomorphisms: changing the definition to have any homomorphism would yield a slightly bigger but semantically equivalent class of queries—though having untamed shapes.

Observe then, by Fact 2.5, that the class $\mathcal{T}\omega_k$ of all C2RPQs of tree-width at most k is closed under refinements and hence under expansions, provided that k is greater or equal to 2. Moreover, $\mathcal{T}\omega_k$ is always closed under subqueries for each k.

Corollary 3.6. For $k \geqslant 2$, for all $C2RPQ \gamma$, $App_{\mathcal{I}\omega_k}(\gamma) \equiv App^{\star}_{\mathcal{I}\omega_k}(\gamma)$.

Example 3.7 (counterexample for k=1). Consider the following query:

$$\gamma(x) \stackrel{\hat{=}}{=} \sqrt[c]{\sum_{b}^{b}}$$

We claim that $\operatorname{App}_{\mathcal{I}\omega_1}(\gamma) \not\subseteq \operatorname{App}_{\mathcal{I}\omega_1}^{\star}(\gamma)$. First, we claim that $\gamma \in \operatorname{Exp}(\operatorname{App}_{\mathcal{I}\omega_1}(\gamma))$ since γ is an expansion of $\delta(x) = x \xrightarrow{abc} x$, which clearly belongs to $\operatorname{App}_{\mathcal{I}\omega_1}(\gamma)$. Then, observe that $\gamma(x)$ has a single refinement: itself! It follows that $\operatorname{App}_{\mathcal{I}\omega_1}^{\star}(\gamma)$ is finite, and consists precisely of all homomorphic images of $\gamma(x)$ of tree-width at most 1, which are:

$$\alpha_{1}(w) = a \subset w \xrightarrow{c} z, \qquad \alpha_{2}(w) = c \subset w \xrightarrow{b} y$$

$$\alpha_{3}(x) = x \xrightarrow{c} w \supset b, \qquad \alpha_{4}(w) = a \subset w \supset c$$

$$\downarrow b$$

which correspond to the case when the following variable are merged: $\{x,y\}$, $\{x,z\}$, $\{y,z\}$ and $\{x,y,z\}$, respectively. Note that all of these queries are CQs, from which it follows that every expansion of a query in $\operatorname{App}_{\mathcal{T}\omega_1}^{\star}(\gamma)$ is one of the α_i , and has a self-loop. In particular, such an expansion cannot have a homomorphism to γ . Hence, we showed that there is an expansion of $\operatorname{App}_{\mathcal{T}\omega_1}(\gamma)$ s.t. no expansion of $\operatorname{App}_{\mathcal{T}\omega_1}(\gamma)$ can be homomorphically mapped to it. Hence, by Proposition 2.4, $\operatorname{App}_{\mathcal{T}\omega_1}(\gamma) \not\subseteq \operatorname{App}_{\mathcal{T}\omega_1}^{\star}(\gamma)$.

In general, by definition, $\operatorname{App}_{\mathcal{I}\omega_k}^{\star}(\gamma)$ is an infinitary union of C2RPQs. Our main technical result shows that, in fact, $\operatorname{App}_{\mathcal{I}\omega_k}^{\star}(\gamma)$ is always equivalent to a *finite* union of C2RPQs. This is done by bounding the length of the refinements occurring in the definition of $\operatorname{App}_{\mathcal{I}\omega_k}^{\star}(\gamma)$. For any $m \geq 1$, we define:

$$\mathrm{App}_{C}^{\star,\leqslant m}(\gamma) = \{\alpha \in C \mid \exists \rho \in \mathrm{Ref}^{\leqslant m}(\gamma), \ \exists f \colon \rho \xrightarrow{hom} \alpha\}.$$

Lemma 3.8 (Key Lemma). For $k \ge 2$ and $C2RPQ \ \gamma$, we have $\operatorname{App}_{\mathcal{J}_{\omega_k}}^{\star}(\gamma) \equiv \operatorname{App}_{\mathcal{J}_{\omega_k}}^{\star \le \ell}(\gamma)$, where $\ell = \Theta(\|\gamma\|_{at}^2 \cdot (k+1)^{\|\gamma\|_{at}})$.

By construction, $\operatorname{App}_{\mathcal{T}_{w_k}}(\gamma)$ is the maximal under-approximation of γ by infinitary unions of C2RPQs of tree-width at most k. Using the equivalence above and Corollary 3.6, it follows that it is also the maximal under-approximation of γ by a UC2RPQ of tree-width at most k.

Corollary 3.9 (Existence of the maximal under-approximation). For each $k \geq 2$, for each class \mathcal{L} closed under sublanguages, and for each query $\Gamma \in \text{UC2RPQ}(\mathcal{L})$, there exists $\Gamma' \in \text{UC2RPQ}(\mathcal{L})$ of tree-width at most k such that $\Gamma' \subseteq \Gamma$, and for every $\Delta \in \text{UC2RPQ}$, if Δ has tree-width at most k and $\Delta \subseteq \Gamma$, then $\Delta \subseteq \Gamma'$. Moreover, Γ' is computable from Γ in ExpSpace.

Proof. The algorithm to compute Γ' is straightforward: it enumerates ℓ -refinements, enumerates its homomorphic images, and keeps the result only if it has tree-width at most k—which can be done in linear time using Bodlaender's algorithm [Bod96, Theorem 1.1].

Using the Key Lemma as a black box—which will be proven in Section 5—, we can now give a proof of the upper bound of Theorem 1.3 for all cases $k \ge 2$ —the case k = 1 will be the object of Section 7.

Lemma 3.10 (Upper bound for Theorem 1.3 for $k \ge 2$). For $k \ge 2$, the semantic tree-width k problem for UC2RPQ is in 2ExpSpace.

Note that $\operatorname{App}_{\mathcal{T}w_k}^{\star \leq \ell}(\gamma)$ has double-exponential size in $\|\gamma\|$, so testing equivalence of γ with this UC2RPQ yields an algorithm in triple-exponential space in $\|\gamma\|$ since (U)C2RPQ equivalence is ExpSpace [CDLV00, Theorem 5]—see also [FLS98, § after Theorem 4.8] for a similar result on CRPQs without inverses but with an infinite alphabet. To get a better upper bound, we first need the following proposition:

Proposition 3.11. The containment problem $\Gamma \subseteq \Delta$ between two UC2RPQs can be solved in non-deterministic space $\Theta(\|\Gamma\| + \|\Delta\|^{c \cdot n_{\Delta}})$, for some constant c, and where n_{Δ} is the maximal number of atoms of a disjunct of Δ , namely $n_{\Delta} = \max\{\|\delta\|_{at} \mid \delta \in \Delta\}$.

Proof. The proposition follows from the following claim.

Claim 3.12 (implicit in [Fig20]). The containment problem $\Gamma \subseteq \Delta$ between two UC2RPQs can be solved in non-deterministic space $\mathcal{O}(\|\Gamma\| + \|\Delta\|^{c \cdot \text{bw}(\Delta)})$, where $\text{bw}(\Delta)$ is the bridgewidth of Δ and c is a constant.

In the statement above, a *bridge* of a C2RPQ is a minimal set of atoms whose removal increases the number of connected components of the query, and the *bridge-width* of a C2RPQ is the maximum size of a bridge therein. The bridge-width of a union of C2RPQs is the maximum bridge-width among the C2RPQs it contains. In particular, the maximal number of atoms of a disjunct is an upper bound for bridge-width.

We provide an alternative upper bound in Proposition B.1 (Appendix B), which also yields a 2ExpSpace upper bound for Lemma 3.10.

Proof of Lemma 3.10. To test whether a query Γ is of semantic tree-width k, it suffices to test the containment $\Gamma \subseteq \Gamma'$, where Γ' is the maximal under-approximation $\bigcup_{\gamma \in \Gamma} \operatorname{App}_{\mathcal{J}w_k}^{\star, \leqslant \ell}(\gamma)$ given by Corollary 3.9: a double-exponential union of single-exponential sized C2RPQs. Thus, by the bound of Proposition 3.11 (and Savitch's Theorem), we obtain a double-exponential space upper bound.

Moreover, from the equivalences $\operatorname{App}_{\mathcal{I}\omega_k}(\gamma) \equiv \operatorname{App}_{\mathcal{I}\omega_k}^{\star}(\gamma)$ and $\operatorname{App}_{\mathcal{I}\omega_k}^{\star}(\gamma) \equiv \operatorname{App}_{\mathcal{I}\omega_k}^{\star \leqslant \ell}(\gamma)$ of Corollary 3.6 and Lemma 3.8, we can derive new characterizations for queries of bounded semantic tree-width.

Theorem 3.13. Assume that \mathcal{L} is closed under sublanguages. For any k > 1 and any query $\Gamma \in UC2RPQ(\mathcal{L})$, the following are equivalent:

- (1) Γ is equivalent to an infinitary union of conjunctive queries of tree-width at most k;
- (2) Γ has semantic tree-width at most k;
- (3) Γ is equivalent to a UC2RPQ(\mathcal{L}) of tree-width at most k.

Proof of Theorem 3.13. The implications $(3) \Rightarrow (2) \Rightarrow (1)$ are straightforward: they follow directly from Fact 2.5. For $(1) \Rightarrow (3)$, note that (1) implies that $\Gamma \equiv \operatorname{App}_{\mathcal{I}_{\omega_k}}(\Gamma)$, and by Lemma 3.8, $\operatorname{App}_{\mathcal{I}_{\omega_k}}(\Gamma) \equiv \Delta = \bigvee_{\gamma \in \Gamma} \operatorname{App}_{\mathcal{I}_{\omega_k}}^{\star, \leqslant \ell}(\gamma)$, so Γ is equivalent to the latter. Since queries of Δ are obtained as homomorphic images of refinements of Γ , all of which are labelled by sublanguages of \mathcal{L} , and since \mathcal{L} is closed under sublanguages, it follows that Γ is equivalent to a UC2RPQ(\mathcal{L}) of tree-width k.

Remark 3.14. The statement of Theorem 3.13 does not hold for k = 1.

- (2) $\not\Rightarrow$ (1) when k=1: consider the CRPQ $\gamma(x,y)=x\xrightarrow{a^*}y\wedge y\xrightarrow{b}x$ of tree-width 1, and hence of semantic tree-width 1, and observe that it is not equivalent to any infinitary union of conjunctive queries of tree-width 1—this can be proven by considering, for example, the expansion $x\xrightarrow{a}z\xrightarrow{a}y\wedge y\xrightarrow{b}x$ of $\gamma(x,y)$ and applying Proposition 2.4.
- (3) $\not\Rightarrow$ (2) when k=1: by [BRV16, Proposition 6.4] the CRPQ of semantic tree-width $1 \gamma(x) = x \stackrel{a}{\leftarrow} z \stackrel{a}{\rightarrow} y \wedge x \stackrel{b}{\rightarrow} y \equiv x \stackrel{ba^-a}{\rightarrow} x$ is not equivalent to any UCRPQ of tree-width 1. Hence, the implication is false when $\mathcal L$ is the class of regular languages over $\mathbb A^\pm$ that do not use any letter of the form a^- .

See Corollary 7.9 for a similar (but different) characterization of queries of semantic tree-width at most 1. As an immediate corollary of Theorem 3.13, by taking \mathcal{L} to be the class of all regular languages over \mathbb{A} , we obtain the following result.

Corollary 3.15. Let $k \ge 2$. A UCRPQ has semantic tree-width at most k if and only if it has one-way semantic tree-width at most k.

Lastly, using Corollary 3.9 as a black box, we can obtain an FPT algorithm for the evaluation problem.

Corollary 3.16 (FPT evaluation for bounded semantic tree-width). For each $k \ge 1$, the evaluation problem for C2RPQs of semantic tree-width at most k is fixed-parameter tractable—FPT—when parametrized in the size of the query. More precisely on input $\langle \Gamma, G \rangle$, the algorithm runs in time $\Theta(f(\|\Gamma\|) \cdot |G|^{k+1} \cdot \log |G|)$ on a Turing machine, where f is a doubly-exponential function—or $\Theta(f(\|\Gamma\|) \cdot |G|^{k+1})$ under a RAM model.

Proof. First, compute from Γ its maximal under-approximation Γ' using Corollary 3.9 in single-exponential space, and hence double-exponential time. Then, evaluate G on Γ' using Proposition 1.1.

This improves the database-dependency from the previously best (and first) known upper bound, which was $\Theta(f'(\|\Gamma\|) \cdot |G|^{2k+1})$ for a single-exponential f' [RBV17, Theorem IV.11 & Lemma IV.13]. We discuss open questions related to this in Section 10.2.

We are left with the proof of the Key Lemma. But before doing so, we will need to introduce in the next Section 4 some basic notions that we will need in the proof, which is deferred to Section 5.

4. Intermezzo: Tagged Tree Decompositions

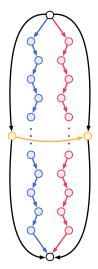
In this section we introduce some technical tools necessary for the proof of the Key Lemma. Remember that its statement deals with

$$\mathrm{App}_{\mathcal{T}w_k}^{\star,\leqslant m}(\gamma) = \{\alpha \in \mathcal{T}w_k \mid \exists \rho \in \mathrm{Ref}^{\leqslant m}(\gamma), \ \exists f \colon \rho \xrightarrow{hom} \alpha\},\$$

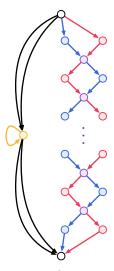
and consequently its proof needs to manipulate homomorphisms from refinements onto C2RPQs of tree-width $\leq k$. The proof will "massage" the homomorphism f and queries α, ρ in order to reduce the size of m, while preserving (a) the existence of a homomorphism between the two queries, (b) the tree-width of the right-hand side, (c) the fact that the left-hand side is a refinement, and (d) some semantic properties of the queries. Our construction will be guided by the tree decomposition of α , and more importantly by how ρ is mapped onto such decomposition.



(A) A query γ of treewidth 3.



(B) A refinement ρ of γ .



(C) A homomorphic image α of ρ of tree-width 2. See Figure 8 for a tree decomposition of α (ignoring the dashed blue lines).

FIGURE 7. An example of a homomorphism $f: \rho \xrightarrow{hom} \alpha$. The strong onto homomorphism f is implicitly defined: it sends the two yellow vertices of ρ on the unique yellow vertex of α , and identifies some blue and red vertices of ρ —thus creating purple vertices in α .

Definition 4.1. Let $f: \rho \xrightarrow{hom} \alpha$ be a homomorphism between two C2RPQs. A *tagged tree decomposition* of f is a triple $(T, \mathbf{v}, \mathbf{t})$ where (T, \mathbf{v}) is a tree decomposition of α , and \mathbf{t} is a mapping \mathbf{t} : Atoms $(\rho) \to V(T)$, called *tagging*, such that for each atom $e = x \xrightarrow{\lambda} y \in \text{Atoms}(\rho)$, we have that $\mathbf{v}(\mathbf{t}(e))$ contains both f(x) and f(y).

In other words, **t** gives, for each atom of ρ , a witnessing bag that contains it, in the sense that it contains the image by f of the atom's source and target. By definition, given a tree decomposition (T, \mathbf{v}) of α and a homomorphism $f : \rho \xrightarrow{hom} \alpha$, there is always one way (usually many) of extending (T, \mathbf{v}) into a tagged tree decomposition of f.

We provide an example of homomorphism $f : \rho \xrightarrow{hom} \alpha$ in Figure 7. Note that in this

We provide an example of homomorphism $f: \rho \xrightarrow{hom} \alpha$ in Figure 7. Note that in this example, ρ is defined as the refinement of a query, and f is strong onto—for now this is innocuous, but we will always work under these assumptions in Section 5. In Figure 8, we give a tagged tree decomposition of this homomorphism. Each bag is given a name, written in the bottom left corner. The tagging is represented as follows: if an atom is tagged in a bag, then it is drawn as a solid bold arrow in this bag. Note that by definition, a given atom is tagged in exactly one bag. For now, blue dashed arrow between bags can be ignored—they will illustrate Definition 4.3.

Fact 4.2. Let $(T, \mathbf{v}, \mathbf{t})$ be a tagged tree decomposition of some strong onto homomorphism $f : \rho \xrightarrow{hom} \alpha$. Let T' be the smallest connected subset of T containing the image of \mathbf{t} . Then $(T', \mathbf{v}|_{T'}, \mathbf{t})$ is still a tagged tree decomposition of f, whose width is at most the width of $(T, \mathbf{v}, \mathbf{t})$.

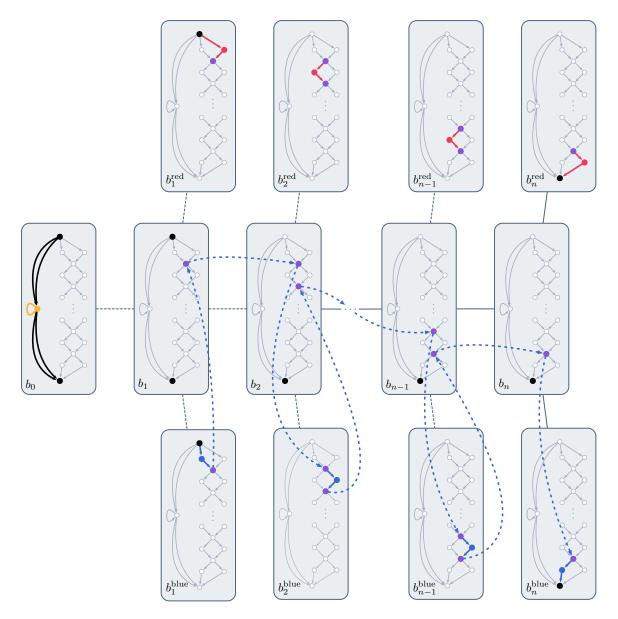


FIGURE 8. A fine tagged tree decomposition of α (see Figure 7) of width 2. (Recall that some bags are omitted for the sake of readability. These bags are there to make the decomposition fine.)

In the following paragraphs, we extend the notion of tagging to paths. We illustrate this notion in Figure 8, where we describe the path induced by the blue path of Figure 7b—which starts at the top-most vertex, follows the blue atoms, and reaches the bottom-most vertex. Informally, in the context of a tagged tree decomposition $(T, \mathbf{v}, \mathbf{t})$ of $f: \rho \xrightarrow{hom} \alpha$, given a path π of ρ , say $x_0 \xrightarrow{\lambda_1} x_1 \xrightarrow{\lambda_2} \cdots \xrightarrow{\lambda_n} x_n$, the path induced by π , denoted by $\mathbf{t}[\pi]$, is informally defined as the following "path" in $T \times \alpha$, seen as a sequence of pairs of bags and variables from $V(T) \times vars(\alpha)$:

- it starts with the bag $\mathbf{t}(x_0 \xrightarrow{\lambda_1} x_1)$ of T and the variable $f(x_0)$ of α ; in Figure 8, this corresponds to bag b_1^{blue} ;
- it then goes to $\langle \mathbf{t}(x_0 \xrightarrow{\lambda_1} x_1), f(x_1) \rangle$;
- it then follows the shortest path in T (unique, since it is a tree) that goes to the bag $\mathbf{t}(x_1 \xrightarrow{\lambda_2} x_2)$, while staying in $f(x_1)$ in α —in Figure 8, this bag is the same as before, namely b_1^{blue} , so we do nothing;
- then, it goes to $\langle \mathbf{t}(x_1 \xrightarrow{\lambda_2} x_2), f(x_2) \rangle$ in a single step;
- it then follows the shortest path in T (unique, since it is a tree) that goes to the bag $\mathbf{t}(x_2 \xrightarrow{\lambda_{\lambda}} x_3)$, while staying in $f(x_2)$ in α —in our running example, we go from b_i^{blue} to b_i , and then to b_{i+1} before reaching b_{i+1}^{blue} ;
- it continues in the same way for all other atoms of the path, ending up with the bag $\mathbf{t}(x_{n-1} \xrightarrow{\lambda_n} x_n)$ and the variable $f(x_n)$ of α .

By construction, note that the constructed sequence $(b_i, z_i)_i$, also denoted by $\binom{b_i}{z_i})_i$, is such that $z_i \in \mathbf{v}(b_i)$. Moreover, the values taken by the sequence $(z_i)_i$ are $(f(x_j))_{0 \leqslant j \leqslant n}$, in the same order but potentially with repetitions. Graphically, this sequence corresponds to a path in the tagged tree decomposition, where one can not only move along the bags, but also along the variables they contain. In our example, the path induced by the blue path of Figure 7b corresponds in Figure 8 to the blue path consisting of both solid and dashed edges. Moreover, note that a single atom $x_0 \xrightarrow{\lambda} x_1$ of ρ induces the path:

$$\left\langle \left(t(x_0 \xrightarrow{\lambda} x_1) \right), \left(t(x_0 \xrightarrow{\lambda} x_1) \right) \right\rangle.$$
 (4.1)

Definition 4.3 (Path induced in a tagged tree decomposition—formal definition). Given a homomorphism $f: \rho \xrightarrow{hom} \alpha$ and a tagged tree decomposition $(T, \mathbf{v}, \mathbf{t})$ of f, the link from an atom $A = x \xrightarrow{\lambda} y$ to an atom $B = y \xrightarrow{\lambda'} z$ of ρ is the unique (possibly empty) sequence $\binom{b_1}{f(y)}, \ldots, \binom{b_n}{f(y)}$, where $\mathbf{t}(A), b_1, \ldots, b_n, \mathbf{t}(B)$ is the unique simple path from $\mathbf{t}(A)$ to $\mathbf{t}(B)$ in T.

The path induced by a path $\pi = x_0 \xrightarrow{\lambda_1} x_1 \xrightarrow{\lambda_2} \cdots \xrightarrow{\lambda_n} x_n$ of ρ is the unique sequence

$$\mathbf{t}[\pi] = \binom{b_0}{f(x_0)} \binom{b_0}{f(x_1)} L_1 \binom{b_1}{f(x_1)} \binom{b_1}{f(x_2)} L_2 \cdots \binom{b_{n-2}}{f(x_{n-2})} L_{n-1} \binom{b_{n-1}}{f(x_{n-1})} \binom{b_{n-1}}{f(x_n)}$$

where $b_i = \mathbf{t}(x_i \xrightarrow{\lambda_{i+1}} x_{i+1})$ and L_i is the link from $x_{i-1} \xrightarrow{\lambda_i} x_i$ to $x_i \xrightarrow{\lambda_{i+1}} x_{i+1}$, for every i.

Moreover, given a bag b of T and a variable z of α , we say that $\mathbf{t}[\pi]$ leaves b at z when $\binom{b}{z}$ belongs to $\mathbf{t}[\pi]$, and this is either the last element of the sequence $\mathbf{t}[\pi]$, or the next element of the sequence has a bag distinct from b.

For example, in Figure 8, $\mathbf{t}[\pi]$ leaves b_1^{blue} at the first purple vertex. Similarly, it leaves b_1 and b_2 at this same vertex. Moreover, it also leaves b_2 at the second purple vertex.

We say that an induced path is *cyclic* if it contains two positions i, j such that $i + 2 \leq j$ and $b_i = b_j$. We say that it is *acyclic* otherwise, meaning that if we visit a bag for the first time, we can visit it again at most once, in which case it must be precisely at the next time step. For instance, the path induced by the blue atom refinement in Figure 8 is cyclic. However, the path induced by a single atom—see (4.1)— is always acyclic.

Fact 4.4. If an induced path $\mathbf{t}[\pi]$ is acyclic, for any bag b, there is at most one variable z of α such that $\mathbf{t}[\pi]$ leaves b at z.

Lastly, we define a fine tagged tree decomposition of $f: \rho \xrightarrow{hom} \alpha$ to be a tagged tree decomposition of f that is also a fine tree decomposition of α . We abuse the notation and

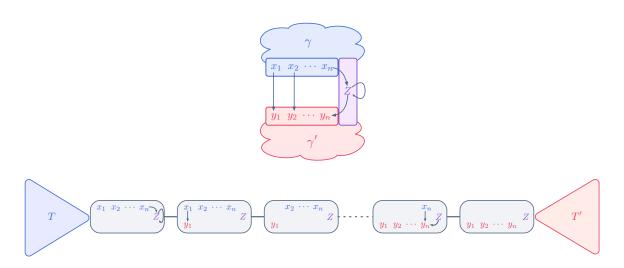


FIGURE 9. The query $\gamma \wedge \gamma' \wedge \delta$ (top) and one of its fine tagged tree decomposition of width at most k (bottom).

talk about the fine tagged tree decomposition of a C2RPQ γ to talk about the fine tagged tree decomposition of the identity homomorphism id: $\gamma \xrightarrow{hom} \gamma$.

One of the key properties of fine tagged tree decompositions is that in any of its nonbranching paths—i.e. paths in T whose non-extremal bags have degree exactly 2—, at least half of the bags are non-full, i.e. they contain at most k variables⁷. Such bags will prove useful in the next section because of the following property.

Proposition 4.5. Let γ, γ' be C2RPQs, and $(T, \mathbf{v}, \mathbf{t})$ —resp. $(T', \mathbf{v}', \mathbf{t}')$ —be a fine tagged tree decomposition of width k of γ —resp. of γ' . Let b, b' be leaves of T and T' respectively, such that b and b' are non-full bags of the same cardinality, and let $Z = \mathbf{v}(b) \cap \mathbf{v}'(b')$. In particular, we have

$$\mathbf{v}(b) = \{x_1, \dots, x_n\} \cup Z \text{ and } \mathbf{v}'(b') = \{y_1, \dots, y_n\} \cup Z,$$

from some variables s.t. the x_i 's are disjoint from the y_i 's. Assume moreover that $vars(\gamma) \cap$ $vars(\gamma') \subseteq Z$. Then, for any conjunction δ of atoms the form:

- $x_i \xrightarrow{L} y_i$ for some $i \in [1, n]$, $x_i \xrightarrow{L} z$ for some $i \in [1, n]$ and $z \in Z$, $z \xrightarrow{L} y_i$ for some $i \in [1, n]$ and $z \in Z$, $z \xrightarrow{L} z'$ for some $z, z' \in Z$,

the query $\gamma \wedge \gamma' \wedge \delta$ has a fine tagged tree decomposition of width k in which the length of the longest non-branching path is smaller than the sum of the longest non-branching paths of T and of T', plus 2n.

The proof of Proposition 4.5 is elementary and illustrated in Figure 9.

Proof. We connect T with T' with $2n \leq 2k$ bags: start from $b_0 = b$, which contains $\{x_1,\ldots,x_n\}\cup Z$. Then create the following bags:

- $\mathbf{v}(b_1) = \{x_1, x_2, \dots, x_n\} \cup \{y_1\} \cup Z = \mathbf{v}(b_0) \cup \{y_1\},$ $\mathbf{v}(b_2) = \{x_2, \dots, x_n\} \cup \{y_1\} \cup Z = \mathbf{v}(b_1) \setminus \{x_1\},$

⁷Recall that in a decomposition of width k, bags are allowed to contain at most k+1 variables.

- $\mathbf{v}(b_{2i-1}) = \{x_i, \dots, x_n\} \cup \{y_1, \dots, y_i\} \cup Z = \mathbf{v}(b_{2i-2}) \cup \{y_i\},\$
- $\mathbf{v}(b_{2i}) = \{x_{i+1}, \dots, x_n\} \cup \{y_1, \dots, y_i\} \cup Z = \mathbf{v}(b_{2i-1}) \setminus \{x_i\}$

for $1 \leq i \leq n$, and observe that $\mathbf{v}(b_{2n}) = \mathbf{v}'(b')$. Then, tag every atom of δ in the first bag of $\langle b_1, \ldots, b_{2n-1} \rangle$ containing both variables of the atom. Such a bag always exists:

- an atom of the form x_i L/Z is tagged in b₀;
 an atom of the form z L/Z z' is tagged in b₀;
 an atom of the form x_i L/Z y_i is tagged in b_{2i-1};
 an atom of the form z L/Z y_i is tagged in b_{2i-1}.

Observe that the decomposition obtained is indeed a fine tagged tree decomposition: in particular, it satisfies that for each variable t, the set of all $b \in T$ containing t is a connected subtree of T, thanks to the assumption that $vars(\gamma) \cap vars(\gamma') \subseteq Z$.

5. Key Lemma: Maximal Under Approximations are Semantically Finite

We can now start to describe the constructions used to prove the Key Lemma 3.8. Given a fixed C2RPQ γ and a fixed $k \ge 1$, we call a *trio* any triple (α, ρ, f) such that $\alpha \in \mathcal{T}\omega_k$ $\rho \in \text{Ref}(\gamma)$ and f is a strong onto homomorphism from ρ to α . For clarity, we will denote such a trio by simply " $f: \rho \xrightarrow{hom} \alpha$ ". Using this terminology, in order to prove Lemma 3.8, it is sufficient (and necessary) to show that:

for every trio
$$f: \rho \xrightarrow{hom} \alpha$$
, there exists another trio $f': \rho' \xrightarrow{hom} \alpha'$ $s.t. \alpha \subseteq \alpha'$ and $\rho' \in \text{Ref}^{\leqslant \ell}(\gamma)$.

Remark 5.1. Note that this section does not use the fact that $k \ge 2$. In particular, Lemma 3.8 holds for k=1. However, Corollary 3.6 does not apply, and $\mathrm{App}_{\mathcal{T}\omega_1}(\gamma)$ (which we are interested in) is not equivalent to $App_{\mathcal{J}_{\omega_1}}^{\star}(\gamma)$ (which is shown to be computable by Lemma 3.8). We discuss this case in further details in Section 7.

5.1. Local Acyclicity. Our first construction, which will ultimately allow us to bound the size of atom refinements, shows that we can assume w.l.o.q. that they induce acyclic paths in a fine tagged tree decomposition of f.

Lemma 5.2. For any trio $f: \rho \xrightarrow{hom} \alpha$, there exists a trio $f': \rho' \xrightarrow{hom} \alpha'$ and a fine tagged tree decomposition $(T', \mathbf{v}', \mathbf{t}')$ of width at most k of f' such that $\alpha \subseteq \alpha'$, $\|\rho'\|_{at} \leqslant \|\rho\|_{at}$ and every atom refinement of ρ' induces an acyclic path in the tree T', in which case we say that $(T', \mathbf{v}', \mathbf{t}')$ is locally acyclic w.r.t. f'.

Note that the fact that f' is a trio implies in particular that ρ' is a refinement of γ . The construction behind Lemma 5.2 is illustrated in Figure 10.

Notation 5.3. When two bags are linked by a dashed edge (as in Figures 8 and 10), it means that there is another bag in between them, which is there to ensure the fact that the decomposition is fine. The vertices contained in this extra bag are exactly the intersection of the vertices contained by its two neighbours, and no atom is tagged inside.

Informal proof of Lemma 5.2. Start with a trio $f: \rho \xrightarrow{hom} \alpha$, and let $(T, \mathbf{v}, \mathbf{t})$ be a fine tagged tree decomposition of f. Consider an atom refinement $\pi = z_0 \xrightarrow{L_1} z_1 \xrightarrow{L_2} \cdots \xrightarrow{L_n} z_n$ in ρ of some atom $x \xrightarrow{L} y$ (with $z_0 = x$ and $z_n = y$), and assume that it induces a cyclic path in T— see e.g. Figure 8. It means that some variables z_i and z_j are mapped by f to the

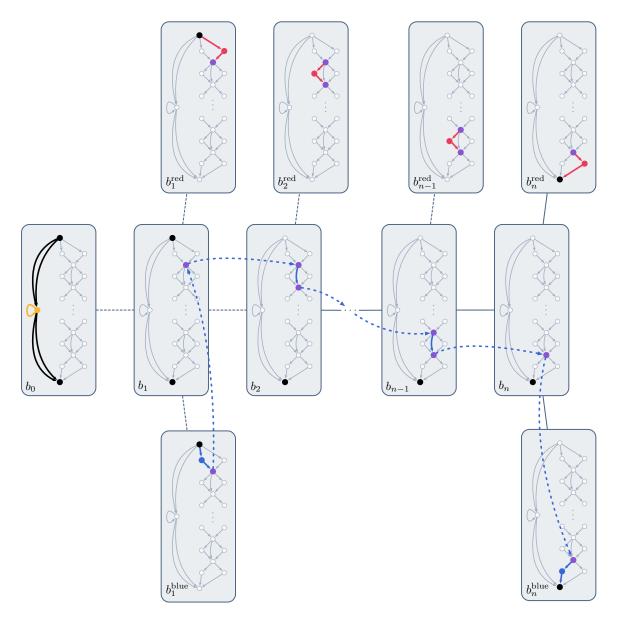


FIGURE 10. Changing the blue atom refinement of γ (see Figure 8) so that it induces an acyclic path.

same bag of T, somewhere along the path induced by π . It suffices then to condense ρ by replacing the atoms $z_i \xrightarrow{L_{i+1}} \cdots \xrightarrow{L_j} z_j$ by a single atom $z_i \xrightarrow{[L_{i+1} \cdots L_j]} z_j$. We thus obtain a new refinement ρ' of γ . Then define α' be simply adding an atom $f(z_i) \xrightarrow{L_{i+1} \cdots L_j} f(z_j)$. The definitions of f' and $(T', \mathbf{v}', \mathbf{t}')$ are then straightforward—potentially, α' should be restricted to the image of $f' : \rho' \xrightarrow{hom} \alpha'$ so that f' is still strong onto by using Fact 4.2. Crucially, $\alpha \subseteq \alpha'$, and α' still has tree-width at most k since we picked $f(z_i)$ and $f(z_j)$ so that they belonged to the same bag of T: therefore, adding an atom between them is innocuous. We then iterate this construction for every atom refinement.

Figure 10 shows the fine tagged tree decomposition $(T', \mathbf{v}', \mathbf{t}')$ obtained by applying the previous construction to the decomposition $(T, \mathbf{v}, \mathbf{t})$ of Figure 8 for the blue atom refinement, followed by applying Fact 4.2. In Figure 8, the induced path was leaving the bag b_2 both at the first and at the second purple vertex. This leads in Figure 10 to a new atom between these vertices. The same phenomenon happens to bags b_3, \ldots, b_{n-1} . Lastly, note that because the atoms tagged in bags $b_2^{\text{blue}}, \ldots, b_{n-1}^{\text{blue}}$ are not in the image of f', these bags were removed by Fact 4.2.

Formal proof of Lemma 5.2. Let π be an atom refinement in ρ that induce a cyclic path in T, say

$$\pi = z_0 \xrightarrow{L_1} z_1 \xrightarrow{L_2} \cdots \xrightarrow{L_{n-1}} z_{n-1} \xrightarrow{L_n} z_n.$$

In order to build the trio $f' : \rho' \xrightarrow{hom} \alpha'$ and a fine tagged tree decomposition T' of f' of width at most k, we will mainly use the fact that if two vertices (u, v) of some graph G belong to the same bag of a tree decomposition (T, \mathbf{v}) of G, then (T, \mathbf{v}) is still also a tree decomposition of the graph obtained by adding an edge from u to v.

By definition, the induced path $\mathbf{t}[\pi] = \begin{pmatrix} b_i \\ x_i \end{pmatrix}_i$ is of the form

$$\mathbf{t}[\pi] = \left\langle \binom{b_{i_0}}{f(z_0)}, \binom{b_{i_0+1}}{f(z_1)}, \dots, \binom{b_{i_1}}{f(z_1)}, \binom{b_{i_1+1}}{f(z_2)}, \dots, \binom{b_{i_{n-1}}}{f(z_{n-1})}, \binom{b_{i_{n-1}+1}}{f(z_n)} \right\rangle,$$

where $i_0 = 0$, and for each l, $b_{i_l} = b_{i_l+1}$. Since it is not acyclic, there exists (j,j') such that $j+2 \leqslant j'$ and $b_j = b_{j'}$. Let n(j) (resp. n(j')) denote the unique index such that $i_{n(j)-1} < j \leqslant i_{n(j)}$ (resp. $i_{n(j')-1} < j' \leqslant i_{n(j')}$). In particular, we have $f(z_{n(j)}) \in \mathbf{v}(b_j)$ and $f(z_{n(j')}) \in \mathbf{v}(b_{j'})$. We claim that n(j) < n(j')—otherwise, we would have twice the same bag in a link, which would contradict the fact that it is a simple path in T.

We can then define

$$\pi' \stackrel{.}{=} t_0 \stackrel{L_1}{\longrightarrow} \cdots \stackrel{L_{n(j)}}{\longrightarrow} t_{n(j)} \stackrel{K}{\longrightarrow} t_{n(j')} \stackrel{L_{n(j')+1}}{\longrightarrow} \cdots \stackrel{L_n}{\longrightarrow} t_n,$$

where $K = [L_{n(j)+1} \cdots L_{n(j')}]$ (see Definition 2.1) and let ρ' be the query obtained from ρ by replacing π with π' . Then, define α' to be the query obtained from α by adding an atom $f(z_{n(j)}) \xrightarrow{K} f(z_{n(j')})$, so that by construction, we have $\alpha \subseteq \alpha'$, that $\rho' \in \text{Ref}(\gamma)$ with $\|\rho'\|_{\text{at}} \leq \|\rho\|_{\text{at}}$ and f induces a homomorphism $f' \colon \rho' \xrightarrow{hom} \alpha'$.

We must then build a tagged tree decomposition $(T', \mathbf{v}', \mathbf{t}')$ of f'. First, we restrict

We must then build a tagged tree decomposition $(T', \mathbf{v}', \mathbf{t}')$ of f'. First, we restrict α' to be the image of $f' \colon \rho' \xrightarrow{hom} \alpha'$, in order to obtain a strong onto homomorphism. Then, starting from the tagged tree decomposition $(T, \mathbf{v}, \mathbf{t})$ of f, restrict \mathbf{t} to the atoms $A \operatorname{toms}(\rho') \setminus \{z_{n(j)} \xrightarrow{K} z_{n(j')}\} \subseteq A \operatorname{toms}(\rho)$, and tag the atom $z_{n(j)} \xrightarrow{K} z_{n(j')}$ to the bag $b_j = b_{j'}$. This tree decomposition has the same width as T. Then, apply Fact 4.2 to get rid of potentially useless bags.

Observe then that the path induced by π' in $(T', \mathbf{v}', \mathbf{t}')$ is simply

$$\mathbf{t}'[\pi'] = \left\langle \binom{b_{i_0}}{f(z_0)}, \binom{b_{i_0+1}}{f(z_1)}, \dots, \binom{b_j}{f(z_{n(j)})}, \binom{b_{j'}}{f(z_{n(j')})}, \dots, \binom{b_{i_{n-1}}}{f(z_{n-1})}, \binom{b_{i_{n-1}+1}}{f(z_n)} \right\rangle$$

and thus $\mathbf{t}'[\pi']$ is strictly shorter than $\mathbf{t}[\pi]$ since $j+2 \leq j'$, by definition of these indices. Finally, observe that if $(T, \mathbf{v}, \mathbf{t})$ is fine then so is $(T', \mathbf{v}', \mathbf{t}')$.

Overall, we built $f' : \rho' \xrightarrow{hom} \alpha'$ together with a fine tagged tree decomposition $(T', \mathbf{v}', \mathbf{t}')$ of width at most k where $\alpha \subseteq \alpha'$ (by Fact 2.2), and $\rho' \in \text{Ref}(\gamma)$ is such that $\|\rho'\|_{\text{at}} \leq \|\rho\|_{\text{at}}$, and for each atom of γ , the refinement of this atom in ρ is exactly the same as the refinement of this atom in ρ' except possibly for one atom, for which the path induced in T' by its refinement in ρ' is strictly shorter than the path induced in T by its refinement in ρ . After

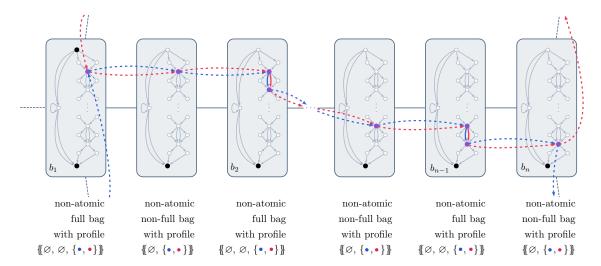


FIGURE 11. Profiles of the bags in the non-branching path between b_1 and b_n in the fine tagged tree decomposition obtained from Figure 8 after applying Lemma 5.2 and Fact 4.2 to both the red and blue atom refinements.

iterating this construction as many times as needed, we obtain a trio as in the conclusion of Lemma 5.2, which concludes our proof.

5.2. **Short Paths.** Ultimately, Lemma 5.2 will allow us to give a bound on the number of leaves of a fine tagged tree decomposition of a trio. The following claim—which is significantly more technical than the foregoing—will give us a bound on the height of a decomposition.

Lemma 5.4. Let $f: \rho \xrightarrow{hom} \alpha$ be a trio and $(T, \mathbf{v}, \mathbf{t})$ be a locally acyclic fine tagged tree decomposition of width at most k of f. Then there is a trio $f': \rho' \xrightarrow{hom} \alpha'$ and a fine tagged tree decomposition $(T', \mathbf{v}', \mathbf{t}')$ of width at most k of f' such that:

- $\alpha \subseteq \alpha'$,
- $(T', \mathbf{v}', \mathbf{t}')$ is locally acyclic w.r.t. f', and
- the length of the longest non-branching path in T is at most $\Theta(\|\gamma\|_{at} \cdot (k+1)^{\|\gamma\|_{at}})$.

To prove Lemma 5.4, we will try to find, in a long non-branching path, some kind of shortcut. The piece of information that is relevant to finding this shortcut is what we call the profile of a bag.

Definition 5.5 (Types and Profiles). Given a trio $f: \rho \xrightarrow{hom} \alpha$ and a fine tagged tree decomposition $(T, \mathbf{v}, \mathbf{t})$ of f, for each bag b of T, we say that:

- b is "atomic" if there is at least one atom $e \in \mathbf{t}^{-1}[b]$ and at least one variable x of e such that $x \in vars(\gamma)$, i.e., the atom e is not in the 'middle' part of an atom refinement;
- otherwise, when b is non-atomic, we assign to each variable $z \in \mathbf{v}(b) \subseteq V(\alpha)$ a type

type $_{z}^{b} = \{x \xrightarrow{L} y \text{ atom of } \gamma \mid \text{the path induced by the atom refinement of } x \xrightarrow{L} y \text{ in } \rho \text{ leaves } b \text{ at } z\},$

where each type is potentially the empty set. Then the *profile* of b is the multiset of the types of z when z ranges over $\mathbf{v}(b)$.

Note that ρ and α can have arbitrarily more atoms than the original query γ , and so the numbers of bags in T can be arbitrarily high. However, only few of them can be atomic: an atom refinement of atom of γ contains at most two atoms with a variable from γ —namely the first and the last atom in the refinement.

Fact 5.6. There is at most $2\|\gamma\|_{at}$ atomic bags in T.

Consider the fine tree decomposition of Figure 10, and now apply the construction of Lemma 5.2 to the red atom refinement, followed by Fact 4.2. We now obtain a non-branching path between bags b_1 and b_n . We depict it in Figure 11: the implicit bags, hidden behind the dashed edges in Figure 10 (see Notation 5.3), are made explicit in this new figure, and, moreover, the rest of the fine tree decomposition is not drawn. Lastly, for each bag, we indicate if it is full and if it is atomic; when it is not atomic, we provide the profile of the bag.

The rest of the proof consists in two parts. First, we show that if two non-atomic bags b and b' occurring in some non-branching path of T have the same profile, then we can essentially replace the path between b and b' by a path of constant length (Claim 5.7). And second, we show that in every sufficiently long non-branching path we can find b and b' satisfying the aforementioned property: this part simply relies on an enhanced "pigeonhole principle" (Fact 5.8).

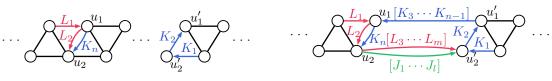
Claim 5.7. Let $f: \rho \xrightarrow{hom} \alpha$ be a trio, and consider a fine tagged tree decomposition of f which is locally acyclic. Suppose there are two bags b and b' such that:

- (1) they contain at most k nodes (i.e., not full bags),
- (2) they have the same profile,
- (3) there is a non-branching path in T between these bags, and
- (4) no bags of the path between b and b' (both included) are atomic.

Then, there exists a trio $f' : \rho' \xrightarrow{hom} \alpha'$ and a fine tagged tree decomposition of f' of width at most k that can be obtained by replacing the non-branching path between b and b' in the fine tagged tree decomposition of f by another non-branching path with at most 2k + 1 bags, such that $\alpha \subseteq \alpha'$.

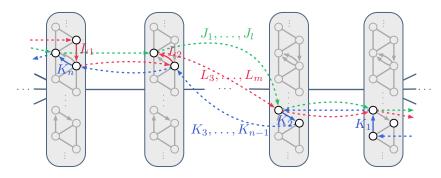
The proof of Claim 5.7 relies on the definition of profile, which was specifically designed so that we can condense every refinement between b and b', while preserving every needed property of the trio. We give first an informal and then a formal proof of Claim 5.7, which are illustrated in Figure 12.

Informal proof of Claim 5.7. If b and b' have the same profile, then in particular they have the same cardinality m, which is smaller or equal to k by assumption. Let $\mathbf{v}(b) = \{x_1, \ldots, x_m\}$ and $\mathbf{v}(b') = \{y_1, \ldots, y_m\}$ be such that: $\operatorname{type}_{x_i}^b = \operatorname{type}_{y_i}^{b'}$ for all $1 \leq i \leq m$. Note that the x_i 's don't need to be distinct from the y_i 's. Essentially, we can then condense every atom refinement in ρ of some atom occurring in a set of the form $\operatorname{type}_{x_i}^b = \operatorname{type}_{y_i}^{b'}$ for some i. At this point, bags strictly comprised between b and b' are discarded, and so are variables of α that do not occur anywhere else. We are left with two halves of a fine tagged tree decomposition that we need to merge, which can easily be done by using Proposition 4.5. The construction makes use of some crucial ingredients to guarantee its correctness.



(A) An approximation α .

(c) The resulting approximation α' .



profile: $\{\{\bullet,\bullet\},\{\bullet\},\varnothing\}$ $\{\{\bullet,\bullet\},\{\bullet\}\}$ $\cdots \quad \{\!\!\{\{\bullet,\bullet\},\{\bullet\}\}\}\!\!\}$ $\{\{\bullet,\bullet,\bullet\},\varnothing,\varnothing\}$

(B) A fine tagged tree decomposition of $f: \rho \xrightarrow{hom} \alpha$ together with the path induced by three atom refinements of ρ (in red, green & blue).

FIGURE 12. A trio $f: \rho \xrightarrow{hom} \alpha$ —where ρ and f are implicit—together with one of its fine tagged tree decomposition (Figures 12a and 12b). There are two non-full bags in the path with the same profile, and thus the query α can be simplified to α' (see Figure 12c) by applying condensations to the atom refinements involved.

- First, an atom $y \xrightarrow{L} y'$ of γ cannot occur in two different types, allowing us to do the condensation of each atom refinement independently—this property is guaranteed by the fact that we started with a locally acyclic fine tagged tree decomposition, so an atom of γ cannot leave a given bag at two different variables, by Fact 4.4.
- Second, this condensation forces us to add new atoms in α (to preserve the existence of a homomorphism from the refinement to the approximation) from some variables of $\mathbf{v}(b)$ to some variables of $\mathbf{v}(b')$, but we only add edges from x_i to y_i , and never from x_i to y_i with $i \neq j$. This allows us to preserve the tree-width of the approximation by using Proposition 4.5.

Formal proof of Claim 5.7. Let

$$\mathbf{v}(b) = \{x_1, \dots, x_m\} \text{ and } \mathbf{v}(b') = \{y_1, \dots, y_m\}$$

be as in the informal proof. Note that given an atom $x \xrightarrow{L} y$ of γ and a bag, there is at most

one variable of α s.t. $x \xrightarrow{L} y$ is in the type of this variable at this bag, by Fact 4.4. For every atom $x \xrightarrow{L} y$ of γ , let $\pi(x \xrightarrow{L} y) = t_0 \xrightarrow{L_1} \dots \xrightarrow{L_n} t_n$ be its refinement in ρ . If $x \xrightarrow{L} y$ is not in some type of the profile of b (or equivalently, of b'), leave it as is. Otherwise, let i (resp. j) be the unique index (by acyclicity) such that $\mathbf{t}[t_0 \xrightarrow{L_1} \dots \xrightarrow{L_n} t_n]$ leaves b at $f(t_i)$ (resp. leaves b' at $f(t_i)$). Define

$$\pi'(x \xrightarrow{L} y) = t_0 \xrightarrow{L_1} \dots \xrightarrow{L_i} t_i \xrightarrow{[L_{i+1} \cdots L_j]} t_j \xrightarrow{L_{j+1}} \dots \xrightarrow{L_n} t_n$$

when $i \leq j$ and otherwise the definition is symmetric. Then, let ρ' be the refinement of γ obtained by simultaneously substituting $\pi(x \xrightarrow{L} y)$ with $\pi'(x \xrightarrow{L} y)$ in ρ , for every atom $x \xrightarrow{L} y$ of γ .

Then, let α' be the query obtained by first adding the atoms

$$f(t_i) \xrightarrow{[L_{i+1}\cdots L_j]} f(t_j),$$

and observe that $f: \rho \xrightarrow{hom} \alpha$ induces a homomorphism $f': \rho' \xrightarrow{hom} \alpha'$ —in particular, note that because of assumption (4) of our claim, we could not have removed images of free variables of γ . Moreover, by construction, $\alpha \subseteq \alpha'$ (by Fact 2.2). As usual, we restrict α' to the image of f' so that it becomes strong onto, while preserving that fact that $\alpha \subseteq \alpha'$. Finally, we build a tagged tree decomposition $(T', \mathbf{v}', \mathbf{t}')$ of f' by applying Proposition 4.5; it can be applied because:

- by assumption (1) and (2) of the claim, both bags have the same cardinality $m \leq k$;
- the variables in common between the first and second half of the decomposition are necessarily included in $Z = \mathbf{v}(b) \cap \mathbf{v}(b')$ since we started from a tree decomposition;
- we only add atoms from x_i to y_i : depending on whether $x_i \in {}^? Z$, and whether $y_i \in {}^? Z$, we fall in one of the four types of atoms allowed by Proposition 4.5.

This concludes the proof of Claim 5.7.

In Figure 13a, we depict the non-branching path (the rest of the fine tree decomposition is not depicted as it is left unchanged) obtained by applying the construction used to prove Claim 5.7 between the second and last bag of Figure 11. Observe that a non-branching path of size $\Theta(n)$ is replaced, by this procedure, by a path with three bags. Then, after applying Fact 4.2, we obtain a trio depicted in Figures 13b to 13d.

Before moving to the proof of Lemma 5.4, we establish one last result.

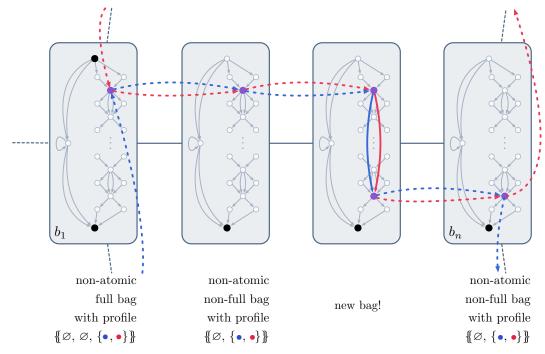
Fact 5.8. Let $n, d, t \in \mathbb{N}$. Let P be a set with at most n elements, and \tilde{P} be the disjoint union of P and $\{\text{trap}, \text{avoid}\}$. For every natural number $m \geq 2(t+1)d(n+1) + 2t$, for every sequence $(p_i)_{0 \leq i < m} \in \tilde{P}^m$ containing at most t elements equal to trap, if at most half of the elements of the sequence are equal to avoid, then there exists i < i' such that $p_i = p_{i'} \neq \text{avoid}$, $i' - i \geq d$ and $p_i \neq \text{trap}$ for every $i \leq j \leq i'$.

Proof. First extract from $(x_i)_{0 \le i < m}$ the subsequence of elements distinct from avoid, of length at least $\lceil \frac{m}{2} \rceil \ge (t+1)d(n+1) + t$. Then extract from it contiguous subsequences that avoid the trap element. Since there is at most t+1 subsequences like this, one of them must have size at least d(n+1). Denote by $(y_i)_{0 \le i < d(n+1)}$ the prefix of such a subsequence. Applying the pigeon-hole principle to $(y_{i\cdot d})_{0 \le i < n+1}$ yields the desired result.

Proof of Lemma 5.4. Let $f: \rho \xrightarrow{hom} \alpha$ be a trio, and $(T, \mathbf{v}, \mathbf{t})$ be a locally acyclic fine tagged tree decomposition of f. If there is a non-branching path $(b_i)_{0 \le i < m}$ in T of length at least m, let $(p_i)_{0 \le i < m}$ be the sequence defined by letting:

$$p_i \stackrel{\circ}{=} \begin{cases} \text{trap} & \text{if } b_i \text{ is atomic,} \\ \text{avoid} & \text{if } b_i \text{ contains } k+1 \text{ variables,} \\ \text{profile of } b_i & \text{otherwise.} \end{cases}$$

Observe that, by Fact 4.4, profiles can be seen encoded as partial functions from the set of atoms of γ to [1,k]—of course this encoding is not surjective—, so there are at



(A) Non-branching path in the "new" fine tagged tree decomposition.

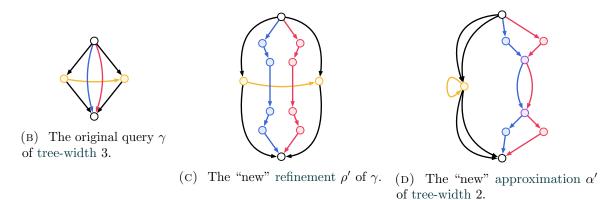


FIGURE 13. Trio resulting from applying Claim 5.7 between the second and last bags of Figure 11.

most $(k+1)^{\|\gamma\|_{at}}$ different profiles on bags with at most k variables. Applying Fact 5.8 for $n=(k+1)^{\|\gamma\|_{at}}, d=2k+1, t=2\|\gamma\|_{at}$ yields, under the assumption that

$$m \geqslant m_0 = 2(2\|\gamma\|_{\text{at}} + 1)(2k+1)((k+1)^{\|\gamma\|_{\text{at}}} + 1) + 4\|\gamma\|_{\text{at}},$$

the existence of indices i < i' such that $i' - i \ge 2k + 1$, and b_i and $b_{i'}$ have the same profile, contain at most k variables, and every bag b_j for $i \le j \le i'$ is non-atomic—note that the hypothesis of Fact 5.8 are satisfied since at most $t = 2\|\gamma\|_{\rm at}$ bags of $(b_i)_{0 \le i < m}$ are atomic (cf. Fact 5.6), and assuming w.l.o.g. that no two consecutive bags of $(b_i)_{0 \le i < m}$ are identical, since the tagged tree decomposition $(T, \mathbf{v}, \mathbf{t})$ of width k is fine, at most half of the bags contain k+1 variables. The assumption $i'-i \ge 2k+1$ means that the path from b_i to $b_{i'}$

has length at least 2k + 2, and thus applying Claim 5.7 will strictly shorten this path. Note that Claim 5.7 preserves the fineness of the tagged tree decomposition, its local acyclicity, and that the size of this tree decomposition is strictly smaller (in number of nodes) than the original tree decomposition. By iteratively applying this construction, we obtain a trio $f' : \rho' \xrightarrow{hom} \alpha'$ together with a locally acyclic fine tagged tree decomposition T' of width at most k, such that $\alpha \subseteq \alpha'$ (by a variation of Fact 2.2) and every non-branching path of T' has length at most $m_0 - 1 \in \mathcal{O}(\|\gamma\|_{\text{at}} \cdot (k+1)^{\|\gamma\|_{\text{at}}})$.

5.3. **Proof of Lemma 3.8.** Finally, our main lemma follows from Lemmata 5.2 and 5.4.

Proof of Lemma 3.8. In order to show $\operatorname{App}_{\mathcal{I}_{w_k}}(\gamma) \subseteq \operatorname{App}_{\mathcal{I}_{w_k}}^{\star,\leqslant \ell}(\gamma)$ —the other containment being trivial—, pick a trio $f : \rho \xrightarrow{hom} \alpha$. Applying Lemma 5.2 and then Lemma 5.4 yields the existence of a trio $f' : \rho' \xrightarrow{hom} \alpha'$ together with a fine tagged tree decomposition $(T', \mathbf{v}', \mathbf{t}')$ of f' such that $\alpha \subseteq \alpha'$ and $(T', \mathbf{v}', \mathbf{t}')$ is locally acyclic, and any non-branching path in T' has length at most $\mathcal{O}(\|\gamma\|_{\operatorname{at}} \cdot (k+1)^{\|\gamma\|_{\operatorname{at}}})$.

Moreover, we can assume w.l.o.g., by applying Fact 4.2, that every leaf of T' is tagged by at least one atom of ρ' . The local acyclicity of T' implies that if b is a leaf of T', and $\pi = x \xrightarrow{L_1} t_1 \xrightarrow{L_2} \cdots \xrightarrow{L_{n-1}} t_{n-1} \xrightarrow{L_n} y$ is an atom refinement in ρ' of some atom $x \xrightarrow{L} y$ of γ , then if b is tagged by one atom of π this atom must either be $z_0 \xrightarrow{L_1} z_1$ or $z_{n-1} \xrightarrow{L_n} z_n$ by local acyclicity. The number of such atoms in ρ' being bounded by $2\|\gamma\|_{\rm at}$, we conclude that T' has at most $2\|\gamma\|_{\rm at}$ leaves.

Then, observe that a tree with at most p leaves and whose non-branching paths have length at most q is of height at most p leaves and whose non-branching paths have $O(\|\gamma\|_{at}^2 \cdot (k+1)^{\|\gamma\|_{at}})$. Using again the local acyclicity of T', observe that the refinement length of p' is at most twice the height of p', and hence $p' \in \operatorname{Ref}^{\leqslant \ell}(\gamma)$ where $\ell = O(\|\gamma\|_{at}^2 \cdot (k+1)^{\|\gamma\|_{at}})$. In other words, $p' \in \operatorname{App}_{\mathcal{J}w_k}^{\star, \leqslant \ell}(\gamma)$. Hence, we have shown that for all $p' \in \operatorname{App}_{\mathcal{J}w_k}^{\star, \leqslant \ell}(\gamma)$, there exists $p' \in \operatorname{App}_{\mathcal{J}w_k}^{\star, \leqslant \ell}(\gamma)$ such that $p' \in \operatorname{App}_{\mathcal{J}w_k}^{\star, \leqslant \ell}(\gamma)$ such that $p' \in \operatorname{App}_{\mathcal{J}w_k}^{\star, \leqslant \ell}(\gamma)$.

This concludes Section 5 and the proof of the Key Lemma. The next four sections are independent of one another:

- in Section 6, we show that the 2ExpSpace complexity of the semantic tree-width k problem can be dropped down to Π_2^p under assumptions on the regular languages;
- in Sections 7 and 8, we adapt the proofs of this section to deal with semantic tree-width 1 and semantic path-width k, respectively.
- in Section 9, we prove an ExpSpace lower bound for the semantic tree-width k problem and semantic path-width k problems;

6. Semantic Tree-Width for Simple Queries

A simple regular expression, or SRE, is a regular expression the form a^* for some letter $a \in \mathbb{A}$ or of the form $a_1 + \cdots + a_m$ for some $a_1, \ldots, a_m \in \mathbb{A}$.

⁸Recall that k is fixed.

⁹The length of a path being its number of nodes, and with the convention that the height of a single node is zero.

Let UCRPQ(SRE) be the set of all UCRPQ whose languages are expressed via SREs. Observe that UCRPQ(SRE) is semantically equivalent to the class of UCRPQs over the closure under concatenation of simple regular expressions since $\gamma(x,y) = x \xrightarrow{e_1 \cdot e_2} y$ is equivalent to $\gamma'(x,y) = x \xrightarrow{e_1} z \wedge z \xrightarrow{e_2} y$. Moreover, UCRPQ(SRE) also corresponds to UC2RPQ whose languages are expressed via SREs; in other words adding two-wayness does not increase the expressivity of the class.

One interest of UCRPQ(SRE) comes from the fact that it is used widely in practice, as recent studies on SPARQL query logs on Wikidata, DBpedia and other sources show that this kind of regular expressions cover a majority of the queries investigated, e.q., 75% of the "property paths" (C2RPQ atoms) of the corpus of 1.5M queries of Bonifati, Martens and Timm [BMT20, Table 15]. An additional interest comes from the fact that the containment problem for UCRPQ(SRE) is much better behaved than for general UCRPQs, since it is in Π_2^p [FGK⁺20, Corollary 5.2], that is, just one level up the polynomial hierarchy compared to the CQ containment problem, which is in NP [CM77], and in sharp contrast with the costly ExpSpace-complete CRPQ containment problem [CDLV00, FLS98].

We devote this section to showing the following result.

Theorem 6.1. For $k \ge 2$, the semantic tree-width k problem for UCRPQ(SRE) is in Π_2^p .

Observe that simple regular expressions are closed under sublanguages. Hence, in the light of Theorem 3.13, the maximal under-approximation of a UCRPQ(SRE) query by infinitary unions of CQs of tree-width k is always equivalent to a UCRPQ(SRE) query of tree-width k. We will see how the construction of the maximal under-approximation of the previous section can be exploited to improve the complexity from 2ExpSpace down to Π_2^p .

- 6.1. Summary Queries. We will first show that the maximal under-approximation of tree-width k of a UC2RPQ can be expressed as a union of polynomial sized "summary" queries. Each summary query represents a union of exponentially-bounded C2RPQs sharing some common structure. Summary queries are normal UC2RPQ queries extended with some special kind of atoms, called "path-l approximations". Intuitively, they represent a maximal under-approximation of tree-width l of queries of the form $\bigwedge_i x_i \xrightarrow{L_i} y_i$ such that $x_i \neq y_j$ for all i, j. Path-l approximations may require an exponential size when represented as UC2RPQs. Formally, a path-l approximation is a query of the form " $P_l(X,Y,\delta)$ " where:
- (1) X, Y, are two disjoint sets of variables of size at most l,
- (2) $\delta(\bar{z})$ is a conjunction of atoms $\bigwedge_{1 \leq i \leq n} A_i$ where \bar{z} contains all variables of $X \cup Y$, (3) each A_i is a C2RPQ atom of the form $x \xrightarrow{L} y$ or $y \xrightarrow{L} x$ such that $x \in X$, $y \in Y$, and L_i is a regular language over A.

We give the semantics of $P_l(X, Y, \delta)$ in terms of infinitary unions of C2RPQs. A query like the one before is defined to be equivalent to the (infinitary) union of all queries $\alpha(\bar{z}) \in \text{App}_{\rho_{w,l}}(\delta)$ such that

 α has a path decomposition of width l where X is the root and Y is the leaf, (6.1)that is, the root and leaf bags contain precisely the vertices of X and Y, respectively. See Figure 14 for an example.

We now simply define a k-summary query as a C2RPQ extended with path-l approximation atoms for any $l \leq k$, with the expected semantics. A refinement of a k-summary query is any C2RPQ obtained by replacing atoms with atom refinements, and each path-l

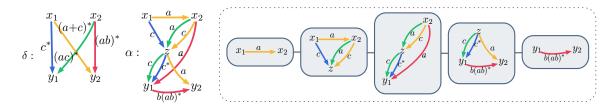


FIGURE 14. Consider the path-l approximation $\mathbf{P}_l(\{x_1, x_2\}, \{y_1, y_2\}, \delta)$ where l = 2 and δ is depicted on the left. Its semantics contains the approximation $\alpha(x_1, x_2, y_1, y_2) \in \mathrm{App}_{\mathscr{P}_{w_l}}(\delta)$ depicted in the middle because it has path decomposition of width l verifying (6.1), as shown on the right.

approximation $P_l(X, Y, \delta)$ with any $\alpha(\bar{z}) \in \operatorname{App}_{\mathcal{P}_{\omega_k}}(\delta)$ verifying (6.1). By definition, a database satisfies a k-summary query if and only if it satisfies one of its refinements.

A tree decomposition of a k-summary query γ consists of a pair (T, \mathbf{v}) with $\mathbf{v} : V(T) \to \mathcal{P}(vars(\gamma))$ such that:

- for every classical atom $x \xrightarrow{L} y$ in γ , there is a bag $b \in T$ such that $\{x, y\} \subseteq \mathbf{v}(b)$;
- for every path-l approximation $\mathbf{P}_l(X, Y, \delta)$ in γ , there are two adjacent bags $b, b' \in T$ such that $X \subseteq \mathbf{v}(b)$ and $Y \subseteq \mathbf{v}(b')$.

The width is defined as usual. Then, by Fact 2.5, we obtain the following upper bound.

Fact 6.2. For any $k \ge 2$, any refinement of a k-summary query with a tree decomposition of width at most k is a C2RPQ of tree-width at most k.

Lastly, a homomorphism from a C2RPQ $\gamma(\bar{z}) = \bigwedge_i x_i \xrightarrow{L_i} y_i$ to a summary query $\delta(\bar{z}') = \left(\bigwedge_j x'_j \xrightarrow{L'_j} y'_j\right) \wedge \left(\bigwedge_{j'} \mathbf{P}_l(X_{j'}, Y_{j'}, \delta_{j'})\right)$ consists of a mapping f from variables of γ to variables of δ such that $f(\bar{z}) = \bar{z}'$, and for each i, there is an atom $f(x_i) \xrightarrow{L_i} f(y_i)$ in δ . Note that if there is a homomorphism from $\gamma(\bar{z})$ to $\delta(\bar{z}')$, then $\delta(\bar{z}') \subseteq \gamma(\bar{z})$.

Let us fix \mathcal{L} to be any class closed under sublanguages. For every $\gamma \in \text{C2RPQ}(\mathcal{L})$, we define $\text{App}_{\mathcal{T}\omega_k}^{\text{zip}}(\gamma)$ as the set of all k-summary queries α such that:

- (a) α has a fine tagged tree decomposition (T, \mathbf{v}) of width at most k,
- (b) there exists a strong onto homomorphism from a refinement ρ of γ to α ,
- (c) T has at most $2\|\gamma\|_{at}$ leaves, and every non-branching path of T consisting only of non-atomic bags must contain at most two non-full bags.

Note that since α is a homomorphic image a refinement of γ , and since \mathcal{L} is closed under sublanguages, then α has only \mathcal{L} -labelled atoms.

Lemma 6.3. Let $k \ge 2$. For every **finite** class \mathcal{L} closed under sublanguages, and for every $\gamma \in \text{C2RPQ}(\mathcal{L})$, we have:

- (1) $\operatorname{App}_{\mathcal{T}\omega_k}^{\operatorname{zip}}(\gamma) \equiv \operatorname{App}_{\mathcal{T}\omega_k}(\gamma),$
- (2) App $_{\mathcal{I}w_k}^{\mathrm{zip}}(\gamma)$ is a union of polynomial-sized k-summary queries having only \mathcal{L} -labelled atoms, and
- (3) one can test in NP if a summary query is part of this union.

Proof. Point (2) follows directly from the definition: there are few branches in the decomposition, branches are short, and each bag cannot contain more than $(k+1)^2 \cdot |\mathcal{L}|$ atoms labelled with \mathcal{L} -languages.

For point (3), recall that one can check if a query has tree-width at most k in linear time, e.g. using Bodlaender's algorithm [Bod96, Theorem 1.1].

To prove (1), notice first that $\operatorname{App}_{\mathcal{T}\omega_k}^{\operatorname{zip}}(\gamma) \subseteq \operatorname{App}_{\mathcal{T}\omega_k}(\gamma)$ as a consequence of Fact 6.2.

For the converse containment, we use Corollary 3.6 and prove instead $\operatorname{App}_{\mathcal{I}\omega_k}^{\star}(\gamma) \subseteq \operatorname{App}_{\mathcal{I}\omega_k}^{\operatorname{zip}}(\gamma)$. Observe that, as corollary of the proof of Lemma 3.8, we can assume to have $\operatorname{App}_{\mathcal{I}\omega_k}^{\star}(\gamma)$ expressed as a union of $\operatorname{C2RPQ}(\mathcal{L})$ with a fine tagged tree decomposition of width k with at most $2\|\gamma\|_{\operatorname{at}}$ leaves, and hence it suffices to replace each non-branching paths having non-atomic bags with path-l approximations.

Indeed, fix a fine tagged tree decomposition and a trio $f: \rho \xrightarrow{hom} \alpha$. Given a long non-branching path from bag b_X with variables X to a bag b_Y with variables Y, such that b_X and b_Y are non-full, and no bag in between is atomic, define $X' = X \setminus Y$ and $Y' = Y \setminus X$. Consider the set S of atoms $u \xrightarrow{L} v$ of γ , such that the path induced $\binom{b_i}{z_i}_i$ by the refinement, say

$$u = w_0 \xrightarrow{L_0} w_1 \xrightarrow{L_1} \cdots \xrightarrow{L_n} w_n = v$$

of $u \xrightarrow{L} v$ in ρ goes through b_X at some variable of X' and through b_Y at some variable of Y', in the sense that $b_i = b_X$ and $z_i \in X'$ for some i, and $b_j = b_Y$ and $z_j \in Y'$ for some j. There exist i', j' such that $f(w_{i'}) = z_i$ and $f(w_{j'}) = z_j$, and w.l.o.g. i' < j'. Now let α' be the query obtained from α by removing all atoms tagged in a bag between b_X and b_Y , and add a path-l approximation query

$$\mathbf{P}_l(X',Y',\delta)$$

where δ is the conjunction over $u \xrightarrow{L} v \in \mathcal{S}$ of $w_{i'} \xrightarrow{[L_{i'} \cdots L_{j'}]} w_{j'}$. Repeat this operation for every non-trivial non-branching path with non-atomic bags. We obtain $\alpha'' \in \operatorname{App}_{\mathcal{I}w_k}^{\operatorname{zip}}(\gamma)$ s.t. $\alpha \subseteq \alpha''$, which concludes the proof that $\operatorname{App}_{\mathcal{I}w_k}^{\star}(\gamma) \subseteq \operatorname{App}_{\mathcal{I}w_k}^{\operatorname{zip}}(\gamma)$.

6.2. **Semantic Tree-Width Problem.** With the previous results in place, we now show that the semantic tree-width k problem is in Π_2^p for UCRPQ(SRE), for every k > 1.

Theorem 6.1. For $k \ge 2$, the semantic tree-width k problem for UCRPQ(SRE) is in Π_2^p .

Proof. It suffices to show the statement for any CRPQ(SRE) γ . Remember that γ is of semantic tree-width k if, and only if, $\gamma \subseteq \text{App}_{\mathcal{I}w_k}^{\text{zip}}(\gamma)$. The first ingredient to this proof is the fact that this containment has a polynomial counterexample property.

Claim 6.4. If $\gamma \not\subseteq \operatorname{App}_{\mathcal{I}w_k}^{\star}(\gamma)$ then there is a polynomial-sized expansion ξ of γ such that $\xi \not\subseteq \operatorname{App}_{\mathcal{I}w_k}^{\star}(\gamma)$.

Proof. Let us call any atom with a language of the form a^* a recursive atom, and any other atom a non-recursive atom. Let n be the number of non-recursive atoms of γ . Hence, any refinement $\rho \in \text{Ref}(\gamma)$ has n atoms deriving from non-recursive atom refinements, all the remaining ones derive from recursive atom refinements.

We will work with the infinitary union of conjunctive queries $\mathcal{U} = \operatorname{App}_{\mathcal{T}w_k}^{\star}(\gamma) \cap \operatorname{CQ}$. Note that $\mathcal{U} = \{\alpha \in \operatorname{CQ} \mid \alpha \in \mathcal{T}w_k \text{ and there is } \xi \in \operatorname{Exp}(\gamma) \text{ s.t. } \xi \xrightarrow{hom} \alpha \}$. It is easy to see that $\mathcal{U} \equiv \operatorname{App}_{\mathcal{T}w_k}^{\star}(\gamma)$ as a consequence of Fact 2.5. By Proposition 2.4, we have $\gamma \not\subseteq \mathcal{U}$ if, and only if, there is some expansion ξ of γ such that $\xi \not\subseteq \mathcal{U}$. In turn, this happens if, and only if, there is no $\delta \in \mathcal{U}$ such that $\delta \xrightarrow{hom} \xi$.

Vol. 21:1

21:36

Take any such counterexample ξ of minimal size (in number of atoms). We show that for any internal path of ξ of the shape

$$\pi = x_0 \xrightarrow{a} x_1 \xrightarrow{a} x_1 \cdots x_{m-1} \xrightarrow{a} x_m,$$

we have $m \leq n+1$. Hence, since ξ is an expansion of a CRPQ(SRE), this means that the size of each *atom expansion*—namely an expansion obtained from a query by only expanding one atom—of ξ is linearly bounded in the size of γ , and thus that ξ is quadratically bounded.

By means of contradiction, if m > n + 1 consider the expansion ξ' resulting from "shrinking" the path π to a path π' of length n+1. Hence, ξ' is smaller than ξ , and since ξ was assumed to be minimal, ξ' cannot be a counterexample. Thus, there is some $\delta \in \mathcal{U}$ such that $f_1: \delta \xrightarrow{hom} \xi'$ for some homomorphism f_1 . Further, by definition of \mathcal{U} , we have $f_2: \xi'' \xrightarrow{hom} \delta$ for some $\xi'' \in \operatorname{Exp}(\gamma)$. Consider then the composition $\xi'' \xrightarrow{hom} \delta \xrightarrow{hom} \xi'$ of f_2 with f_1 and let us call it $g: \xi'' \xrightarrow{hom} \xi'$. By definition of n there must be at least one atom $x_i \xrightarrow{a} x_{i+1}$ of the shrunken path π' of ξ' which either (i) is not in the image of f_1 , or (ii) all its g-preimages proceed from atoms $z \xrightarrow{a} z'$ of ξ'' which are in the expansions of recursive atoms of γ . We show that, in both cases, we can replace $x_i \xrightarrow{a} x_{i+1}$ with a path of a's of any arbitrary length l > 0, obtaining a conjunctive query ξ'_{+l} which is—still—not a counterexample. In the first case (i), we actually obtain that $\delta \xrightarrow{hom^+} \xi'_{+l}$. In the second case (ii), we have to replace each atom $z \xrightarrow{a} z'$ in the g-preimage of $x_i \xrightarrow{a} x_{i+1}$ in ξ'' by an a-path of length l, obtaining some expansion ξ''_{+l} of γ . We also replace each atom in the f_1 -preimage of $x_i \xrightarrow{a} x_{i+1}$ by an a-path of length l obtaining some δ_{+l} such that $\xi''_{+l} \xrightarrow{hom} \delta_{+l} \xrightarrow{hom} \xi'_{+l}$. Further, $\delta_{+l} \in \mathcal{I}\omega_k$ since $\mathcal{I}\omega_k$ is closed under refinements by Fact 2.5. In both cases this shows that ξ'_{+l} is not a counterexample. In particular, for l=m-n-1, we have $\xi'_{+l}=\xi$, and this would contradict the fact that ξ is a counterexample. Therefore, there exists a counterexample of polynomial (quadratic) size whenever $\gamma \not\subseteq \operatorname{App}_{\mathcal{T}_{W_{\iota}}}^{\star}(\gamma)$.

The second ingredient is that testing whether a CQ is a counterexample is in co-NP.

Claim 6.5. The problem of testing, given a C2RPQ γ and a CQ ξ , whether $\xi \subseteq \text{App}_{\mathcal{I}w_k}^{\text{zip}}(\gamma)$, is in NP.

Proof. We first guess a polynomial-sized k-summary query δ_{zip} and test in NP that it is part of $\text{App}_{\mathcal{T}_{W_k}}^{\text{zip}}(\gamma)$ by Lemma 6.3. Let us call Δ be the equivalent UCRPQ(SRE) query, given by Lemma 6.3 cum Lemma 3.8. We have to check that there is some expansion δ of Δ such that there is a homomorphism $\delta \xrightarrow{hom} \xi$. We first guess a valuation $\mu : vars(\delta_{\text{zip}}) \to vars(\xi)$. Now it remains to check that:

- (1) For every CRPQ atom $x \xrightarrow{a^*} y$ of δ_{zip} there is an a-path in ξ from $\mu(x)$ to $\mu(y)$.
- (2) Every path-l approximation $\mathbf{P}_l(X,Y,\bigwedge_{1\leqslant i\leqslant n}A_i(x_i,y_i))$ of δ_{zip} contains a CQ δ_{path} admitting a path decomposition of width l which starts with the bag X and ends with Y. And further, there is a homomorphism $h:\delta_{\mathrm{path}}\xrightarrow{hom}\xi$ which coincides with μ on variables $X\cup Y$.

Observe that these two properties hold true if, and only if, there is some expansion δ of Δ such that $\delta \xrightarrow{hom} \gamma$. It is clear the first point can be achieved in polynomial time (actually, in NL) since it is a simple reachability query. The second point can also be achieved in polynomial time (or in NL), since the fine path decomposition of width l can be guessed on-the-fly using l+1 pointers to the variables of γ (cf. Lemma 8.10). An NL algorithm can advance down the path decomposition while simultaneously

(1) guessing the conjunctive query δ_{path} via its fine path decomposition of width k,

- (2) checking that there is a partial homomorphism to γ (*i.e.*, a homomorphism from the subquery of γ restricted to current bag's variables to γ),
- (3) ensuring that the CQ δ_{path} being built is an element of $\mathbf{P}_l(X,Y,\bigwedge_{1\leqslant i\leqslant n}A_i(x_i,y_i))$, which requires to also guess a homomorphism $\rho \xrightarrow{hom} \delta_{\text{path}}$ from a refinement ρ of $\bigwedge_{1\leqslant i\leqslant n}A_i(x_i,y_i)$.

Further, a simple test can ensure that the first and last bags of the decomposition coincide with the guessed assignment μ . Since the number of pointers (bounded by k+1) is fixed, this subroutine is in NL, and hence in polynomial time. This yields an NP algorithm for testing $\xi \subseteq \operatorname{App}_{\mathcal{J}_{WL}}^{\operatorname{zip}}(\gamma)$.

As a consequence of the two claims, we obtain a Σ_2^p algorithm for non-containment of $\gamma \subseteq \operatorname{App}_{\mathcal{I}\omega_k}^{\operatorname{zip}}(\gamma)$: We first guess an expansion ξ of γ of polynomial size, and we then test $\xi \not\subseteq \operatorname{App}_{\mathcal{I}\omega_k}^{\operatorname{zip}}(\gamma)$ in co-NP. This gives a Π_2^p algorithm for the semantic tree-width k problem, which is correct by Lemma 6.3 and Claim 6.4.

7. Acyclic Queries: the Case k=1

Observe that in the previous sections we have treated the cases of semantic tree-width kfor every $k \ge 2$. However, the case k = 1 remains rather elusive so far. While the Key Lemma holds for k=1, it proves the computability of an object that is irrelevant to study semantic tree-width 1, see Remark 5.1. The problem comes from Example 3.7, namely that $\operatorname{App}_{\mathcal{T}_{w_1}}(\gamma) \not\equiv \operatorname{App}_{\mathcal{T}_{w_1}}^{\star}(\gamma)$. This is the main obstacle why our approach does not directly yield an algorithm for the case k=1, which had been previously solved by Barceló, Romero and Vardi [BRV16]. However, as we argue in this section, a rather elegant modification on the notion of tree-width allows to use our approach as a unifying framework for both the case k=1 and the cases $k \ge 2$. Concretely, we introduce a family of classes $\{Ctw_k\}_k$ such that $\operatorname{App}_{\mathcal{H}w_k}(\gamma) \equiv \operatorname{App}_{\mathcal{C}tw_k}^{\star}(\gamma)$ for every γ and k, and where $\operatorname{App}_{\mathcal{C}tw_1}^{\star}(\gamma) \equiv \operatorname{App}_{\mathcal{C}tw_1}^{\star}(\gamma)$. As a corollary, we reprove [BRV16, Theorem 6.1], namely that the semantic tree-width 1 problem is ExpSpace-complete. Further, we can also solve the one-way semantic tree-width 1 problem, which is outside the scope of [BRV16]. Remember that for k=1, the semantic tree-width and one-way semantic tree-width 1 problems are two independent problems, since there are queries of semantic tree-width 1 but not of one-way semantic tree-width 1 (cf. Remark 3.14).

7.1. Contracted Tree-Width. We next formally define the notion of "contracted tree-width", meaning the tree-width of the graph obtained by contracting paths (or directed paths) into edges. This altered notion of tree-width will allow us to seamlessly prove the case of k = 1 for Theorem 1.3.

Given a C2RPQ γ , an *internal path* is a sequence of atoms¹⁰

$$x_0 \stackrel{L_1}{\rightleftharpoons} x_1 \stackrel{L_2}{\rightleftharpoons} \cdots \stackrel{L_{n-1}}{\rightleftharpoons} x_{n-1} \stackrel{L_n}{\rightleftharpoons} x_n$$

where each x_i for $i \in [1, n-1]$ has total degree exactly 2 and is existentially quantified. Its contraction is defined as the edge

$$x_0 \xrightarrow{K_1 \cdot K_2 \cdots K_{n-1} \cdot K_n} x_n,$$

¹⁰We write $x \rightleftharpoons y$ to mean that there is either an atom $x \stackrel{\lambda}{\rightarrow} y$ or an atom $x \stackrel{\lambda}{\leftarrow} y$.

where $K_i = L_i$ if the atom between x_i and x_{i+1} is directed from left to right, and $K_i = L_i^-$ if the atom is directed from right to left.¹¹

Similarly, a one-way internal path is a sequence of atoms

$$x_0 \xrightarrow{L_1} x_1 \xrightarrow{L_2} \cdots \xrightarrow{L_{n-1}} x_{n-1} \xrightarrow{L_n} x_n$$

where each x_i for $i \in [1, n-1]$ has exactly in-degree and out-degree 1 in γ and is existentially quantified. Its *one-way contraction* is defined as the edge

$$x_0 \xrightarrow{L_1 \cdot L_2 \cdots L_{n-1} \cdot L_n} x_n$$
.

A contraction (resp. one-way contraction) of a C2RPQ is any query obtained by iteratively replacing some internal paths (resp. one-way internal paths) by their contraction (resp. one-way contraction). By definition, a query is always equivalent to any of its contractions or one-way contractions.

Definition 7.1. Define the contracted tree-width (resp. one-way contracted tree-width) of a C2RPQ as the minimum of the tree-width among its contractions (resp. of its one-way contractions). Let Ctw_k and $1Ctw_k$ be, respectively, the set of all C2RPQs of contracted tree-width at most k and of CRPQs of one-way contracted tree-width at most k.

For instance, the query

$$\gamma(x_0, x_1) \stackrel{\hat{=}}{=} \begin{array}{c} x_0 \xrightarrow{K} x_1 \\ \downarrow \\ y \end{array}$$

has contracted tree-width one since the internal path $x_0 \xrightarrow{L} y \xleftarrow{M} x_1$ can be contracted into $x_0 \xrightarrow{LM^-} x_1$. On the other hand, its one-way contracted tree-width is two, since there is no non-trivial one-way internal path as x_1 is an output variable.

Note that, by definition:

- the contracted tree-width is at most the one-way contracted tree-width, which is in turn at most the tree-width;
- for $k \ge 2$, these notions collapse (by Fact 2.5);
- for k = 1, both inequalities can be strict.

Moreover, for any $k \ge 1$, contracted tree-width at most k and one-way contracted tree-width at most k are both closed under refinements: if a query has tree-width at most k, so does any refinement thereof. In fact, the CQs of contracted tree-width 1 precisely correspond to what in [BRV16, §5.2.1, p1358] is known as "pseudoacyclic graph databases".

Fact 7.2. Let $k \ge 1$. For any CRPQ γ , we have $\operatorname{App}_{1\mathcal{T}\omega_k}(\gamma) \equiv \operatorname{App}_{1\mathcal{C}t\omega_k}^{\star}(\gamma)$. Moreover, for any C2RPQ γ , $\operatorname{App}_{\mathcal{T}\omega_k}(\gamma) \equiv \operatorname{App}_{\mathcal{C}t\omega_k}^{\star}(\gamma)$.

$$\operatorname{App}_{\mathcal{T}w_k}(\gamma) \equiv \operatorname{App}_{\mathcal{C}tw_k}(\gamma)$$
 since contractions preserve semantics,
 $\equiv \operatorname{App}_{\mathcal{C}tw_k}^*(\gamma)$ by Observation 3.5.

The same arguments work with one-wayness.

¹¹Given a regular language L over \mathbb{A}^{\pm} , we define a regular language L^- over \mathbb{A}^{\pm} by induction on regular expressions: $\emptyset^- = \emptyset$, $(a)^- = a^-$, $(a^-)^- = a$, $(L_1 \cdot L_2)^- = L_2^- \cdot L_1^-$, $(L^*)^- = (L^-)^*$ and $(L_1 + L_2)^- = L_1^- + L_2^-$. Then, for any graph, there is a path from x to y labelled by a word of L iff there is a path from y to x labelled by a word of L^- .

7.2. The Key Lemma for Contracted Tree-Width One. We show next that contracted tree-width 1 has all the needed properties for the analogue of Key Lemma for k = 1 to hold.

Lemma 7.3. For any CRPQ γ , we have $\operatorname{App}_{1Ct\omega_1}^{\star}(\gamma) \equiv \operatorname{App}_{1Ct\omega_1}^{\star,\leqslant \ell_1}(\gamma)$, where $\ell_1 = \Theta(\|\gamma\|_{at}^3)$. Similarly, for a C2RPQ γ , $\operatorname{App}_{Ct\omega_1}^{\star}(\gamma) \equiv \operatorname{App}_{Ct\omega_1}^{\star,\leqslant \ell_1}(\gamma)$.

Proof. Consider the proof of the Key Lemma (Lemma 3.8). We claim that:

- (1) the constructions of Lemmata 5.2 and 5.4 both preserve contracted tree-width at most 1 and one-way contracted tree-width at most 1;
- (2) the upper bound $\ell \in \mathcal{O}(\|\gamma\|_{at}^2 \cdot 2^{\|\gamma\|_{at}})$ can be easily boiled down to $\ell_1 \in \mathcal{O}(\|\gamma\|_{at}^3)$ in the special case of k = 1.
- (1) **Preservation of contracted tree-width.** We claim that all constructions of Section 5 preserve contracted tree-width at most 1. The setting is similar, except that now, a trio consists of a triple $f: \rho \to \alpha$ where ρ is a refinement of a fixed C2RPQ γ , and α is a C2RPQ of *contracted* tree-width 1. We now apply the constructions not to a decomposition of α but to a fine tagged tree decomposition of a *contraction* of α of tree-width 1.
- **Fact 7.4.** Let γ be a C2RPQ, χ be a contraction of γ , and $(T, \mathbf{v}, \mathbf{t})$ be a fine tagged tree decomposition of χ of width at most 1. Let $z, z' \in \mathbf{v}(b)$ for some bag $b \in T$. Then $\gamma \wedge z \xrightarrow{\lambda} z'$ still has contracted tree-width at most 1.

As a consequence, the construction of Lemma 5.2—which takes us from Figure 8 to Figure 10—preserves contracted tree-width 1. Then, Proposition 4.5—illustrated in Figure 9—can be trivially adapted to our setting as follows:

Fact 7.5. Let γ , γ' be two C2RPQ with a disjoint set of variables. Let z (resp. z') be a variable of γ (resp. γ'). If both γ and γ' have contracted tree-width at most 1, then so does $\gamma \wedge \gamma' \wedge z \xrightarrow{\lambda} z'$.

As a consequence, the construction of Lemma 5.4—which takes us from Figure 10 to Figure 13—preserves contracted tree-width 1.

(2) **Improved upper bound.** In the proof claiming that in a sufficiently long non-branching path, we can always find two non-full, non-atomic bags with the same profile (see the proof of Lemma 5.4), we obtain a bound of $\mathcal{O}(2^{\|\gamma\|_{\mathrm{at}}})$. We actually claim that it can be improved to obtain a polynomial bound. This is because, for width 1, a non-full bag b contains exactly 1 variable z_b . So, its profile consists simply on a set of atoms of γ —namely the set of atoms whose refinement induces a path which leaves the bag b at z_b . But we claim that in a non-branching path, not all of these $2^{\|\gamma\|_{\mathrm{at}}}$ profiles can occur at the same time. Indeed, in tree decompositions, the set of bags containing a given variable must be connected. This property can be lifted to paths in tagged tree decompositions in the following way.

Fact 7.6. Let $(T, \mathbf{v}, \mathbf{t})$ be a tagged tree decomposition of some homomorphism $f : \rho \xrightarrow{hom} \alpha$. Let π be a path in ρ . Assume that:

- the simple path in T from b to b'' goes through b',
- there exists some variable z of α such that $\mathbf{t}[\pi]$ leaves b at z, and
- there is no variable like that for the bag b'.

Then, there is no variable z of α such that $\mathbf{t}[\pi]$ leaves b'' at z.

Proof of Fact 7.6. Fix a tagged tree decomposition $(T, \mathbf{v}, \mathbf{t})$ of some homomorphism $f: \rho \xrightarrow{hom} \alpha$ and π be a path in ρ . Let b, b', b'' be bags such that the simple path in T from b to b''

goes through b'. Say that an induced path $\mathbf{t}[\pi] = (\binom{b_i}{z_i})_i$ visits a bag b if $b_i = b$ for some i. Note that this is equivalent to saying that there exists a variable z of α s.t. $\mathbf{t}[\pi]$ leaves b at z. Hence, Fact 7.6 boils down to the following property: if $\mathbf{t}[\pi]$ visits both b and b", then it must also visit b'. This property holds because by construction, the sequence $(b_i)_i$ —namely the projection of $\mathbf{t}[\pi]$ onto T—is a path in T, with some node repetition.

As a consequence, if an atom occurs in a bag, but not in a latter one, then it can never occur again. Hence, the number of bags of size 1 in a non-branching path where each bag has a different profile must be at most $n = \|\gamma\|_{at}$. Hence, Fact 5.8 yields a bound of $\mathcal{O}(\|\gamma\|_{at}^2)$. Finally, we can conclude like in Section 5.3: we obtain a tree with at most $\mathcal{O}(\|\gamma\|_{at})$ leaves, and with non-branching paths of length at most $\mathcal{O}(\|\gamma\|_{at}^2)$, so the tree has size at most $\ell_1 \in \mathcal{O}(\|\gamma\|_{at}^3)$. By local acyclicity, this concludes the proof of Lemma 7.3. The case of one-way contracted tree-width is completely similar.

Lemma 7.7. Let $k \geqslant 1$.

- (1) Given a UCRPQ Γ , it has one-way semantic tree-width at most 1 iff $\Gamma \equiv \operatorname{App}_{1\mathcal{C}Iw_1}^{\star,\leqslant \ell_1}(\Gamma)$; (2) Given a UC2RPQ Γ , it has semantic tree-width at most 1 iff $\Gamma \equiv \operatorname{App}_{\mathcal{C}tw_1}^{\star,\leqslant \ell_1}(\Gamma)$; where $\ell_1 \in \mathcal{O}(\|\gamma\|_{at}^3)$.

Proof. To prove the first point:

• if Γ is equivalent to a UCRPQ Δ of tree-width at most 1, then $\Delta \subseteq \mathrm{App}_{\mathcal{I}\omega_1}(\Gamma)$ and by Fact 7.2 and Lemma 7.3, $\Delta \subseteq \operatorname{App}_{\mathbb{C}^{t_{w_1}}}^{\star, \leq \ell_1}(\Gamma)$, and hence:

$$\Gamma \equiv \Delta \subseteq \operatorname{App}_{1Ctw_1}^{\star, \leqslant \ell_1}(\Gamma) \subseteq \Gamma.$$

• If $\Gamma \equiv \operatorname{App}_{1Ctw_1}^{\star,\leqslant \ell_1}(\Gamma)$, then Γ is equivalent to a UCRPQ of contracted tree-width at most 1, and hence (by contraction) it is equivalent a UCRPQ of tree-width at most 1.

The second point can be proven similarly.

Corollary 7.8 (Upper bound of Theorem 1.3 for k=1). The semantic tree-width 1 problem and one-way semantic tree-width 1 problem are in ExpSpace.

Proof. The fact that the semantic tree-width 1 problem is in ExpSpace is actually the main result of [BRV16, Theorem 6.1], but we show how the upper bound follows as a direct corollary of Lemma 7.7 above. Since $\ell_1 \in \Theta(\|\gamma\|_{at}^3)$, $\operatorname{App}_{ct\omega_1}^{\star,\leqslant \ell_1}(\gamma)$ is an exponential union of polynomial sized C2RPQs, and thus by Proposition 3.11 the containment problem $\Gamma \subseteq \operatorname{App}_{\mathcal{C}t\omega_1}^{\star,\leqslant \ell_1}(\Gamma)$ is in ExpSpace, and so is the semantic tree-width 1 problem (since the converse containment $\operatorname{App}_{\mathcal{C}t\omega_1}^{\star,\leqslant \ell_1}(\Gamma) \subseteq \Gamma$ always holds, cf . Remark 3.2). The proof for one-way semantic tree-width 1 problem is analogous

Lastly, note that we can derive from Lemma 7.3 a characterization of semantic tree-width 1 somewhat similar to Theorem 3.13.

Corollary 7.9. Assume that \mathcal{L} is closed under sublanguages.

Two-way queries: For any query $\Gamma \in UC2RPQ(\mathcal{L})$, the following are equivalent:

- (1) Γ is equivalent to an infinitary union of conjunctive queries of contracted tree-width at most 1:
- (2) Γ has semantic tree-width at most 1;
- (3) Γ is equivalent to a UC2RPQ(\mathcal{L}) of contracted tree-width at most 1;

(4) Γ is equivalent to a UC2RPQ(\mathcal{L}') of tree-width at most 1, where \mathcal{L}' is the closure of \mathcal{L} under concatenation and inverses, i.e. \mathcal{L}' is the smallest class containing \mathcal{L} and such that if $K, L \in \mathcal{L}'$ then $K \cdot L \in \mathcal{L}'$ and $K^- \in \mathcal{L}'$.

One-way queries: Similarly, if $\Gamma \in UCRPQ(\mathcal{L})$, then the following are equivalent:

- (1) Γ is equivalent to an infinitary union of conjunctive queries of one-way contracted tree-width at most 1;
- (2) Γ has one-way semantic tree-width at most 1;
- (3) Γ is equivalent to a UCRPQ(\mathcal{L}) of one-way contracted tree-width at most 1;
- (4) Γ is equivalent to a UCRPQ(\mathcal{L}') of tree-width at most 1, where \mathcal{L}' is the closure of \mathcal{L} under concatenation, i.e. \mathcal{L}' is the smallest class containing \mathcal{L} and such that if $K, L \in \mathcal{L}'$ then $K \cdot L \in \mathcal{L}'$.

Note in particular how point (4) of each characterization reflects that a UCRPQ of semantic tree-width 1 can have one-way semantic tree-width at least 2—as we showed in Remark 3.14. More generally, the differences between this last corollary and Theorem 3.13 highlight the different combinatorial behaviour that semantic tree-width k has, depending on whether k = 1 or k > 1.

Remark 7.10. Finally, note that results of Sections 6 and 7 can be joined in order to show that the semantic tree-width 1 problems are decidable in Π_2^p for UC2RPQs over the closure under concatenation and inverses of SREs (resp. for UCRPQs over the closure under concatenation of SREs).¹²

8. Semantic Path-Width

In this section, we extend our results to path-width. Our motivation lies in the fact that UC2RPQs of bounded semantic path-width admit a paraNL¹³ algorithm for the evaluation problem—see Theorem 8.9—to be compared with FPT for bounded semantic tree-width.

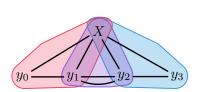
8.1. Path-Width of Queries. Recall that for tree-width, for any $k \ge 2$, we proved that a CRPQ is equivalent to a finite union of C2RPQs of tree-width at most k iff it is equivalent to finite union of CRPQs of tree-width at most k (Theorem 3.13). In other words, two-way navigation does not help to minimize further the semantic tree-width of a query that does not use two-way navigation. This property does not hold for k = 1 (Remark 3.14). We show in Remark 8.2 that it also does not hold for path-width, no matter the value of $k \ge 1$.

This motivates the following two definitions:

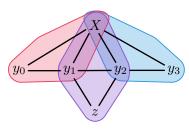
- the semantic path-width of a UC2RPQ is the minimal path-width of a UC2RPQ equivalent to it.
- the *one-way semantic path-width* of a UCRPQ is the minimal path-width of a UCRPQ equivalent to it.

¹²While this the whole class of UCRPQs over SREs has the same expressivity as UCRPQs over the closure under concatenation of SREs, this is not true if one adds the constraint of having tree-width at most 1, see Corollary 7.9.

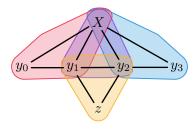
¹³This is the parametrized counterpart of non-deterministic logspace.



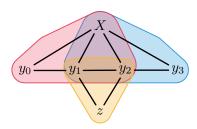
(A) Graph G_k with a path decomposition of width k, with three bags.



(B) Expansion G'_k of G_k with a path decomposition of width k+1, with three bags.



(C) Tree decomposition of G'_k of width k, with four bags.



(D) Path decomposition of G'_k of width k+1, with three bags.

FIGURE 15. The class of multigraphs with path-width at most $k \ge 1$ is not closed under expansions: illustration of a multigraph \mathcal{G}_k of path-width k (Figure 15a) whose expansion \mathcal{G}'_k has path-width k+1 (Figures 15b and 15d)—but tree-width k (Figure 15c). Set X represents a (k-1)-clique.

For a given UCRPQ, the two natural numbers are well-defined, and the former is always less or equal to the letter. The *semantic path-width* k *problems* ask, given a UCRPQ (resp. UC2RPQ), if it has semantic path-width (resp. one-way semantic path-width) at most k.

In this section, we first show that the semantic path-width k problems are decidable (Theorem 8.7), and then after showing that evaluation of UC2RPQs of bounded path-width is NL (Lemma 8.10) we deduce that for the evaluation problem for UC2RPQs of bounded semantic path-width (in particular, this captures the case of UCRPQs of bounded one-way semantic path-width) is in paraNL when parametrized in the size of the query (Theorem 8.9).

8.2. **Deciding Bounded Semantic Path-Width.** The key (implicit) ingredient in the proof of Theorem 3.13 and Corollary 3.9 is that tree-width at most k is closed under expansions (Fact 2.5). Unfortunately, this property fails for path-width.

Fact 8.1. For each $k \ge 1$, the class of graphs of path-width at most k is not closed under expansions.

The counterexample is illustrated in Figure 15. A formal proof can be found in Appendix C.

Remark 8.2. Contrary to the case of semantic tree-width, for every k there are CRPQs which are of semantic path-width k but not of one-way semantic path-width k.

Proof. Indeed, let

$$\gamma_{k}(\bar{x}, \bar{y}) = \left(\bigwedge_{1 \leq i < j \leq k-1} x_{i} \xrightarrow{a} x_{j} \right) \wedge \left(\bigwedge_{1 \leq i \leq k-1} \bigwedge_{0 \leq j \leq 3} x_{i} \xrightarrow{b} y_{i} \right)$$
$$\wedge \left(\bigwedge_{0 \leq j < 3} y_{i} \xrightarrow{c} y_{i+1} \right) \wedge y_{1} \xrightarrow{d} z \wedge y_{2} \xrightarrow{e} z,$$

whose underlying graph corresponds to Figure 15b. Observe that it is a core and that only z is existentially quantified. Then in $\gamma_k(\bar{x},\bar{y})$, one can replace the two atoms $y_1 \stackrel{d}{\to} z \wedge y_2 \stackrel{e}{\to} z$ by $y_1 \stackrel{de^-}{\to} y_2$, while preserving the semantics. The underlying graph of this new query being Figure 15a, it shows that γ_k has semantic path-width k.

Finally, we claim that γ_k has one-way semantic path-width k+1. The upper bound follows from Figure 15d. For the lower bound, consider a UCRPQ $\Delta_k(\bar{x}, \bar{y})$ such that $\gamma_k \equiv \Delta_k$. Since γ_k is a CQ, the equivalence implies that there exists an expansion ξ of a CRPQ of Δ_k such γ_k and ξ are homomorphically equivalent. Since γ_k is a core, it follows that ξ contains it as a subgraph. Hence, the underlying directed multigraph of the CRPQ in Δ_k from which ξ originated must contain a one-way contraction of ξ as a subgraph. But the only one-way contraction of ξ is itself, and so it follows that at least one CRPQ in Δ_k contains the underlying graph of ξ as a subgraph. Therefore, Δ_k has path-width at least k+1, which concludes the proof that the one-way semantic path-width of γ_k is at least (and hence exactly) k+1.

As done for contracted tree-width, we define contracted path-width.

Definition 8.3. Define the contracted path-width (resp. one-way contracted path-width) of a C2RPQ as the minimum of the path-width among its contractions (resp. of its one-way contractions). Let Cpw_k and $1Cpw_k$ be, respectively, the set of all C2RPQs of contracted path-width at most k and of CRPQs of one-way contracted path-width at most k.

The statements and proofs of this section are analogous to the ones of Section 7 in the context of contracted tree-width 1. We keep the order and structure to make this correspondence evident.

Again, by definition, contracted path-width at most k and one-way contracted path-width at most k are both closed under refinements: if a query has width at most k, so does any refinement thereof.

Fact 8.4. Let $k \ge 1$. For any CRPQ γ , we have $\operatorname{App}_{1\mathcal{O}_{W_k}}(\gamma) \equiv \operatorname{App}_{1\mathcal{C}_{PW_k}}^{\star}(\gamma)$. Moreover, for any C2RPQ γ , $\operatorname{App}_{\mathcal{O}_{W_k}}(\gamma) \equiv \operatorname{App}_{\mathcal{C}_{PW_k}}^{\star}(\gamma)$.

Proof.

$$\operatorname{App}_{1\mathcal{O}_{\omega_k}}(\gamma) \equiv \operatorname{App}_{1\mathcal{O}_{\mathcal{O}_{\omega_k}}}(\gamma)$$
 since contractions preserves the semantics, $\equiv \operatorname{App}^{\star}_{1\mathcal{O}_{\mathcal{O}_{\omega_k}}}(\gamma)$ by Observation 3.5.

The same arguments work for C2RPQs.

Lemma 8.5. For $k \geqslant 1$ and $CRPQ \ \gamma$, we have $\operatorname{App}^{\star}_{1Cpw_k}(\gamma) \equiv \operatorname{App}^{\star,\leqslant \ell}_{1Cpw_k}(\gamma)$, where $\ell = \Theta(\|\gamma\|^2_{at} \cdot (k+1)^{\|\gamma\|_{at}})$. Similarly, for a $C2RPQ \ \gamma$, $\operatorname{App}^{\star}_{Cpw_k}(\gamma) \equiv \operatorname{App}^{\star,\leqslant \ell}_{Cpw_k}(\gamma)$.

Proof. Consider the proof of the Key Lemma (Lemma 3.8): both constructions (Lemmata 5.2 and 5.4) preserve the contracted path-width of α if the operations are applied to a suitable path decomposition of a contraction of α of width k.

Lemma 8.6. Let $k \geqslant 1$.

- (1) Given UCRPQ Γ , it has one-way semantic path-width at most k iff $\Gamma \equiv \operatorname{App}_{\mathcal{L}pw_k}^{\star,\leqslant \ell}(\Gamma)$; (2) Given a UC2RPQ Γ , it has semantic path-width at most k iff $\Gamma \equiv \operatorname{App}_{\mathcal{L}pw_k}^{\star,\leqslant \ell}(\Gamma)$.

Proof. To prove the first point:

• if γ is equivalent to a UCRPQ Δ of path-width at most k, then $\Delta \subseteq \operatorname{App}_{\mathcal{P}_{w_k}}(\gamma)$ and by Fact 8.4 and Lemma 8.5, $\Delta \subseteq \operatorname{App}_{1C_{PW_{k}}}^{\star,\leqslant \ell}(\gamma)$, and hence:

$$\gamma \equiv \Delta \subseteq \operatorname{App}_{1\mathcal{C}_{\mathcal{DW}_h}}^{\star, \leqslant \ell}(\gamma) \subseteq \gamma.$$

• If $\gamma \equiv \operatorname{App}_{1Cpw_k}^{\star,\leqslant \ell}(\gamma)$, then γ is equivalent to a UCRPQ of contracted path-width at most k, and hence it is equivalent a UCRPQ of path-width at most k.

The second point can be proven similarly.

We can now prove the main theorem.

Theorem 8.7. For each $k \ge 1$, the semantic path-width k problems are decidable. Moreover, they lie in 2ExpSpace and are ExpSpace-hard. Moreover, if k = 1, these problems are in fact ExpSpace-complete.

Proof. The upper bounds follow from Lemma 8.6. The lower bounds will be shown in Lemma 9.1. Lastly, to prove the ExpSpace upper bound for k=1, we can apply the same trick as in Corollary 7.8.

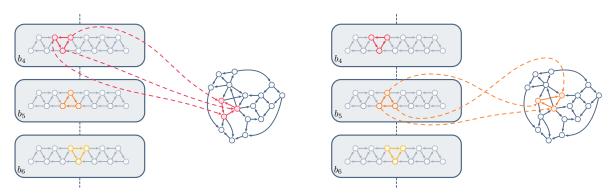
Similarly to Corollary 7.9, we can derive from Lemma 8.5 a characterization of semantic path-width at most k.

Corollary 8.8. Assume that \mathcal{L} is closed under sublanguages, and let $k \geq 1$. **Two-way queries:** For any query $\Gamma \in UC2RPQ(\mathcal{L})$, the following are equivalent:

- (1) Γ is equivalent to an infinitary union of conjunctive queries of contracted path-width at most k;
- (2) Γ has semantic path-width at most k;
- (3) Γ is equivalent to a UC2RPQ(\mathcal{L}) of contracted path-width at most k;
- (4) Γ is equivalent to a UC2RPQ(\mathcal{L}') of path-width at most k, where \mathcal{L}' is the closure of \mathcal{L} under concatenation and inverses, i.e. \mathcal{L}' is the smallest class containing \mathcal{L} and such that if $K, L \in \mathcal{L}'$ then $K \cdot L \in \mathcal{L}'$ and $K^- \in \mathcal{L}'$.

One-way queries: Similarly, if $\Gamma \in UCRPQ(\mathcal{L})$, then the following are equivalent:

- (1) Γ is equivalent to an infinitary union of conjunctive queries of one-way contracted path-width at most k;
- (2) Γ has one-way semantic path-width at most k;
- (3) Γ is equivalent to a UCRPQ(\mathcal{L}) of one-way contracted path-width at most k;
- (4) Γ is equivalent to a UCRPQ(\mathcal{L}') of path-width at most k, where \mathcal{L}' is the closure of \mathcal{L} under concatenation, i.e. \mathcal{L}' is the smallest class containing \mathcal{L} and such that if $K, L \in \mathcal{L}'$ then $K \cdot L \in \mathcal{L}'$.



- (A) Partial homomorphism computed at the fourth step of the algorithm.
- (B) Partial homomorphism computed at the fifth step of the algorithm.

FIGURE 16. Algorithm to evaluate C2RPQs of path-width at most k (here k=2) in non-deterministic logspace. Each subfigure represents: (i) on the left-hand side, a path decomposition of a C2RPQ, (ii) on the right-hand side, a graph database, and (iii) a partial homomorphism from the C2RPQ to the database.

8.3. Evaluation of Queries of Bounded Semantic Path-Width. In this section, we show that, as a consequence of Theorem 8.7, we can obtain an efficient algorithm for the evaluation problem.

Theorem 8.9. For each $k \ge 1$, the evaluation problem, restricted to UC2RPQs of semantic path-width at most k is in paraNL when parametrized in the size of the query. More precisely, the problem, on input $\langle \Gamma, G \rangle$, can be solved in non-deterministic space $f(|\Gamma|) + \log(|G|)$, where f is a single exponential function.

The class paraNL was introduced in [CCDF97, Definition, p. 123] under the name "uniform NL + advice". It was renamed paraNL in [FG03, Definition 1, p. 294]. For the sake of simplicity, instead of either of those definitions, we use the characterization of paraNL proven in [FG03, Theorem 4, p. 296].

We define paraNL as the class of parametrized languages $L \subseteq \Sigma^* \times \mathbb{N}$ for which there is a Turing machine M s.t.

$$M ext{ accepts } \langle x, k \rangle ext{ iff } \langle x, k \rangle \in L,$$
 input parameter

and, moreover, M runs in non-deterministic space $f(k) + \mathcal{O}(\log(|x|))$, where $f: \mathbb{N} \to \mathbb{N}$ is a computable function. A typical example of paraNL problem is the model-checking problem for first-order logic on finite structures, when parametrized by the maximum degree of the structure [FG03, Example 6].

To show Theorem 8.9, we first focus on the evaluation of queries of bounded path-width.

Lemma 8.10. For each $k \ge 1$, the evaluation problem, restricted to UC2RPQs of path-width at most k, is NL-complete.

Proof. Lower bound. NL-hardness directed follows from the NL-hardness of the reachability problem in directed graphs, see *e.g.* [AB09, Theorem 4.18, p. 89].

Upper bound, first part: with the path decomposition. First, we assume that a tagged path decomposition of width at most k of the query of is also provided as part of the input. Moreover, we assume w.l.o.g. that the input is C2RPQ—the extension to UC2RPQ being straightforward. So, we are given as input:

- a database together with a tuple of nodes $G(\bar{u})$,
- a C2RPQ $\gamma(\bar{x})$, and
- a tagged path decomposition $\langle T, \mathbf{v}, \mathbf{t} \rangle$ of width at most k of $\gamma(\bar{x})$.

The algorithm, illustrated in Figure 16, maintains a partial homomorphism $f: X \to G$ of these variables onto G. We scan the bags of the decomposition from left to right.

- Initially—before even scanning the first bag—f is the map with empty domain.
- Then, when scanning the *i*-th bag b_i , we start by restricting f to variables of dom $(f) \cap b_i$. Then, we extend f so that it is defined on the whole bag b_i . For every variable g in $b_i \setminus \text{dom}(f)$:
 - if it belongs to \bar{x} , say $y = x_i$, we let $f(x_i) = u_i$;
 - otherwise, we non-deterministically guess the value of f(y).

We then check, for every atom $x \xrightarrow{L} y$ of $\gamma(\bar{x})$ which is tagged in the current bag b_i if there is a path from f(x) to f(y) labelled by a word of L in G. If not, we reject.

If the algorithm manages to scan the whole bag decomposition without rejecting, it accepts. Completeness of the algorithm is trivial. Correctness follows from the fact that if a variable occurs in bags b_i and b_k with $i \leq k$, then it must also belong to every bag b_j for $j \in [i,k]$. As a consequence, a variable x is assigned exactly one value f(x) during the whole process.

Concerning the space complexity:

- By construction, at the *i*-th step of the algorithm, f is defined exactly on b_i , so on at most k+1 variables. So, f can be stored in space $(k+1)\log(|G|)$;
- we need a counter with $\log(|T|)$ bits to scan through the tagged path decomposition,
- each atomic check—checking if there is an L-labelled path from f(x) to f(y)—can be done in non-deterministic space $c \cdot (\log(|G|) + \log(|\mathcal{A}_L|))$, where \mathcal{A}_L is an NFA for L, using a straightforward adaptation of the NL algorithm for graph connectivity; note that these atomic checks are independent of one another, so we can reuse this space.

Overall, the algorithm runs in non-deterministic space $\mathcal{O}(k \log(|G|) + \log(|T|)) = \mathcal{O}(\log(|G|) + \log(|T|))$, which is logarithmic in the size of the input.

Upper bound, second part: without the path decomposition. Then, we claim that the original problem—when the tagged tree decomposition is not part of the input—also lies in NL. This is because one can compute, from γ , a path decomposition in (deterministic) logarithmic space by ¹⁴ [KM10, Theorem 1.3, p. 2]. Then, a path decomposition can be turned into a tagged path decomposition in (deterministic) logarithmic space by tagging an atom $x \xrightarrow{L} y$ in the first bag containing both x and y. The conclusion follows since functions computable in non-deterministic logarithmic space are closed under composition [AB09, Lemma 4.17, p. 88].

¹⁴This result is an adaption of a similar statement for tree-width [EJT10, Theorem I.1, p. 143]. Note that the promise that the query has bounded path-width—in fact bounded tree-width suffices—in a crucial assumption of [EJT10, Theorem I.1, p. 143].

We can now conclude with Theorem 8.9, namely that the evaluation problem for UC2RPQs of semantic path-width k is in paraNL.

Proof of Theorem 8.9. Given a UC2RPQ $\Gamma(\bar{x})$ of semantic path-width at most k and a database $G(\bar{u})$, we first compute $\operatorname{App}_{1C\rho\omega_k}^{\star,\leqslant\ell}(\Gamma)$ —where $\ell=\Theta(\|\Gamma\|_{\operatorname{at}}^2\cdot(k+1)^{\|\Gamma\|_{\operatorname{at}}})$ —, which is equivalent to Γ by Lemma 8.6. Then, we use Lemma 8.10 to evaluate each $\delta(\bar{x})\in\operatorname{App}_{1C\rho\omega_k}^{\star,\leqslant\ell}(\Gamma)$ on $G(\bar{u})$. If one of the queries accepts, we accept. Otherwise, we reject.

The non-deterministic space needed by the algorithm is:

- $\Theta(\ell)$ bits to enumerate and store $\delta(\bar{x})$, where $\ell = \Theta(\|\Gamma\|_{at}^2 \cdot (k+1)^{\|\Gamma\|_{at}})$
- $\mathcal{O}(\log |G| + \log |\delta|) \subseteq \mathcal{O}(\log |G| + \log |\ell| + \log |\Gamma|)$ to evaluate $\delta(\bar{x})$ on $G(\bar{u})$, by Lemma 8.10 and since $||\delta|| \leq ||\Gamma|| \cdot \ell$.

Overall, we use non-deterministic space $f(\|\Gamma\|) + \mathcal{O}(\log(|G|))$ where f is a single exponential, which concludes the proof.

9. Lower Bounds for Deciding Semantic Tree-Width and Path-Width

An ExpSpace lower bound follows by a straightforward adaptation from the ExpSpace lower bound for the case k = 1 [BRV16, Proposition 6.2].

Lemma 9.1 (Lower bound of Theorem 1.3). For every $k \ge 1$, the following problems are ExpSpace-hard, even if restricted to Boolean CRPQs:

- the semantic tree-width k problem;
- the one-way semantic tree-width k problem;
- the semantic path-width k problem:
- the one-way semantic path-width k problem.

We say that a C2RPQ is *connected* when its underlying undirected graph is connected. We first give a small useful fact.

Fact 9.2 (Implicit in [BRV16, Proof of Proposition 6.2]).

- (1) Let G, G' be two databases and δ be a connected Boolean C2RPQ. If the disjoint union G + G' (i.e., the union assuming V(G) and V(G') are disjoint) satisfies δ , then either G satisfies δ or G' satisfies δ .
- (2) Let γ, δ be Boolean C2RPQs. If δ is connected and $\gamma \subseteq \delta$, then there exists a subquery γ' of γ , obtained as connected component of γ , such that $\gamma' \subseteq \delta$.

Notice first that if γ and δ are CQs then the proof of Fact 9.2 follows directly from the equivalence of $\gamma \subseteq \delta$ (resp. G satisfies γ) and the existence of a homomorphism from δ to γ (resp. γ to G).

Proof. We first prove the second point. Write $\gamma = \gamma_1 \wedge \ldots \wedge \gamma_n$ where $\gamma_1, \ldots, \gamma_n$ are connected components of γ , and assume by contradiction that for all $i, \gamma_i \not\subseteq \delta$. Then there exists a database G_i such that G_i satisfies γ_i but not δ . Consider the disjoint union $G = G_1 + \ldots + G_n$.

On the one hand, since the γ_i 's have disjoint variables and G_i satisfies γ_i for each i, then G satisfies γ . On the other hand, G cannot satisfy δ : if there was a homomorphism from δ to G, since δ is connected, there would exist an index i such that δ is mapped on G_i , which would contradict the fact that G_i does not satisfy δ . Hence, G does not satisfy δ , which contradicts the containment $\gamma \subseteq \delta$.

To prove the first point, we simply apply the second one, by letting γ be the conjunction of the canonical CQ associated with G and G'—which is in fact the canonical CQ associated with G + G'. From the assumption that G + G' satisfies δ it follows that $\gamma \subseteq \delta$ and so, by the first point, there is either a homomorphism from δ to G or from δ to G'.

We can then prove Lemma 9.1.

Proof of Lemma 9.1. Fix $k \ge 1$. We focus on semantic tree-width, but the exact same reduction works for the other three problems. We introduce an intermediate problem, called the asymmetric containment problem for tree-width k: given two Boolean CRPQs γ and γ' , where γ has tree-width k, γ' is connected and does not have semantic tree-width k, it asks whether $\gamma \subseteq \gamma'$. The proof of the lemma then contains two parts:

- (1) first, we reduce the asymmetric containment problem for tree-width k to the semantic tree-width k problem,
- (2) then, we prove that the asymmetric containment problem for tree-width k is ExpSpacehard.

(1): We reduce the instance (γ, γ') of the asymmetric containment problem for tree-width k to the instance $\gamma \wedge \gamma'$ of the semantic tree-width k problem. We simply have to check that $\gamma \subseteq \gamma'$ if and only if $\gamma \wedge \gamma'$ has semantic tree-width k. The left-to-right implication is straightforward since $\gamma \subseteq \gamma'$ implies that $\gamma \wedge \gamma' \equiv \gamma$ and γ was assumed to have tree-width k. For the converse implication, if $\gamma \wedge \gamma' \equiv \delta$ where δ is a UC2RPQ of tree-width k then write $\delta = \bigvee_{i=1}^{n} \delta_i$ where the δ_i 's are C2RPQs and let $\delta_{i,1}, \ldots, \delta_{i,k_i}$ be the connected components of δ_i .

Since for each i we have $\delta_i \subseteq \delta \equiv \gamma \land \gamma' \subseteq \gamma'$, by Fact 9.2, there exists j_i such that $\delta_{i,j_i} \subseteq \gamma'$. Let $\delta' = \bigvee_{i=1}^n \delta_{i,j_i}$ so that, by construction $\delta' \subseteq \gamma'$. However, note that δ' has tree-width at most k but γ' was assumed not to have semantic tree-width k, hence $\delta' \subsetneq \gamma'$, so there exists G' such that:

$$G'$$
 satisfies γ' and G' does not satisfy δ' . (9.1)

We now prove that $\gamma \subseteq \gamma'$. Let G be a database satisfying γ . Then the disjoint union G + G' satisfies $\gamma \wedge \gamma'$ since G satisfies γ , G' satisfies γ' and γ and γ' are Boolean so we can assume w.l.o.g. that they have disjoint variables. As a consequence, G + G' satisfies δ and hence δ' , so there exists i such that G + G' satisfies δ_{i,j_i} . Since δ_{i,j_i} is connected, either G satisfies δ_{i,j_i} or G' satisfies δ_{i,j_i} . By Equation (9.1), the latter cannot hold, so G satisfies δ_{i,j_i} and hence γ' .

Therefore, we have shown that for each database G that satisfies γ , then G satisfies γ' , i.e., $\gamma \subseteq \gamma'$. Overall, $\gamma \wedge \gamma'$ has semantic tree-width k if and only if $\gamma \subseteq \gamma'$.

(2): We now show that the asymmetric containment problem for tree-width k is ExpSpace-hard. It was shown in [Fig20, Lemma 8] that the containment of CRPQs was still ExpSpace-hard when restricted to inputs of the form:

$$\gamma() = \bullet \xrightarrow{K} \bullet \qquad \subseteq ? \qquad \bullet \underbrace{\vdots}_{L_p} \bullet = \delta(),$$

where K, L_1, \ldots, L_p are regular languages over \mathbb{A} . We reduce it to the following problem:

$$\gamma'() = \bullet \xrightarrow{K} \stackrel{\#}{\circ} \qquad \subseteq ? \qquad \bullet \xrightarrow{\stackrel{L_1}{:}} \bullet \xrightarrow{\mathbb{A}^*} \bullet \stackrel{\#}{\longrightarrow} \stackrel{\#}{\longrightarrow} \bullet = \delta'().$$

where the right-hand side of δ' is a directed (k+2)-clique and where # is a new symbol, i.e. $\# \notin \mathbb{A}$.

We claim that $\gamma \subseteq \delta$ if and only if $\gamma' \subseteq \delta'$. The forward implication is direct and the converse implication simply relies on the fact that $\# \notin \mathbb{A}^{15}$. Then, observe that γ' has tree-width $1 \leq k$, and that δ' is connected but do not have semantic tree-width at most k.

To prove the last point, consider a UC2RPQ Δ'' that is equivalent to δ' . Pick any expansion ξ'_1 of δ' . Since $\Delta'' \subseteq \delta'$, there exists an expansion ξ'' of Δ'' such that there is a homomorphism from ξ'_1 to ξ'' . Dually, since $\delta' \subseteq \Delta''$, there exists an expansion ξ'_2 of δ' such that there is a homomorphism from $\xi'' \to \xi'_2$. Overall, we have homomorphisms $\xi'_1 \to \xi'' \to \xi'_2$. Since ξ'_1 and ξ'_2 are both expansions of δ' , they contain a #-labelled directed (k+2)-clique, and the #-letter appears nowhere else. Should the homomorphism $\xi'_1 \to \xi''$ not be injective, ξ'' would contain a #-labelled self-loop, and hence, the homomorphism $\xi'' \to \xi'_2$ would yield a #-self loop in ξ'_2 , which does not exist! Hence, the homomorphism from ξ'_1 to ξ'' is injective on the (k+2)-clique. As a result, ξ'' contains a (k+2)-clique and has tree-width at least k+1. We conclude that Δ'' has tree-width at least k+1 by Fact 2.5, provided that $k \geqslant 2$.

Hence, we have shown that $\gamma \subseteq \delta$ if and only if $\gamma' \subseteq \delta'$ where γ' has tree-width at most k, where δ' is connected and has semantic tree-width at least k+1. Since our reduction can be implemented in polynomial time, we conclude that the problems of Lemma 9.1 are ExpSpace-hard.

10. Discussion

10.1. Complexity. We have studied the definability and approximation of UC2RPQ queries by queries of bounded tree-width and shown that the maximal under-approximation in terms of an infinitary union of conjunctive queries of tree-width k can be always effectively expressed as a UC2RPQ of tree-width k (Corollary 3.9). However, while the semantic tree-width 1 problem is shown to be ExpSpace-complete (which was also established in [BRV16, Theorem 6.1, Proposition 6.2]), we have left a gap between our lower and upper bounds in Theorem 1.3 for every k > 1.

Question 10.1. For k > 1, is the semantic tree-width k problem ExpSpace-complete?

A related question is whether the containment problem between a C2RPQ and a summary query is in ExpSpace. Should this be the case, then the semantic tree-width k problem would be in ExpSpace. We also point out that since every path-l approximation can be expressed by a polynomial UC2RPQ of tree-width 2k—this is the same idea as in [RBV17, Lemma IV.13]—, one can produce, for every UC2RPQ Δ a union Γ of poly-sized C2RPQ of tree-width 2k such that $\mathrm{App}_{\mathcal{T}_{Wk}}(\Delta) \subseteq \Gamma \subseteq \Delta$. This implies that the following

¹⁵Indeed, the only possible homomorphisms from expansions of δ' to expansions of γ' are the ones sending the expansions of atoms containing L_1, \ldots, L_p inside the expansion of the atom on K.

"promise" problem¹⁶ is decidable in ExpSpace: given a UC2RPQ Γ, answer 'yes' if Γ is of semantic tree-width 2k, and answer 'no' if Γ is not of semantic tree-width k. The fact that $App_{\mathcal{T}w_k}(\Delta)$ can be approximated by an exponential query of tree-width 2k+1 can also be seen as a corollary of the proof of [RBV17, Theorem V.1].

We also do not know whether the Π_2^p bound on the semantic tree-width k problem for UCRPQ(SRE) has a matching lower bound. The known lower bound for the UCRPQ(SRE) containment problem [FGK⁺20, Theorem 5.1] does not seem to be useful to be employed in a reduction in this context, since it necessitates queries of arbitrary high tree-width.

10.2. Characterization of Tractability. Our result implies that for each k the evaluation problem for UC2RPQs Γ of semantic tree-width k is fixed-parameter tractable—or FPT—taking the query as parameter, *i.e.*, in time $\mathcal{O}(|G|^c \cdot f(|\Gamma|))$ for a computable function f and constant c, where G is the database given as input. While this was a known fact [RBV17, Corollary IV.12], the dependence on the database was c = 2k + 1. Our results show that the dependence can be improved to c = k + 1, similarly to [BRV16, Theorem 6.3] for the case k = 1. It has been further shown by Feier, Gogacz and Murlak that the evaluation can be done with a single-exponential f [FGM24, Theorem 22].

In a similar vein, our results show that the evaluation problem for UC2RPQs of semantic path-width k is in paraNL. It is unknown whether the semantic bounded width properties characterize all FPT and paraNL classes.

Question 10.2. Does every recursively enumerable class of CRPQs with paraNL evaluation have bounded semantic path-width?

Question 10.3 (Also mentioned in [RBV17, §IV-(4)]). Does every recursively enumerable class of CRPQs with FPT evaluation have bounded semantic tree-width?

Note that the classes of bounded contracted path-width or contracted tree-width are not counterexamples to Questions 10.2 and 10.3, since the path-width is upper-bounded by one plus the contracted path-width, and lower-bounded by the contracted path-width—and similarly for tree-width—and so a width is bounded *iff* its contracted variant is bounded.

In the case of CQs, the answer is 'yes' to Question 10.3 [Gro07, Theorem 1] under standard complexity-theoretic hypotheses ($W[1] \neq \mathsf{FPT}$). For Question 10.2, the answer is still 'yes' [CM13, Theorem 3.1] conditional to a less standard assumption¹⁷ (no Tree-hard problem is in paraNL).

However, attempting at answering these questions for CRPQs is considerably more challenging. In particular, one important technical difficulty is that a class of CRPQs with unbounded tree-width may contain queries with no expansions which are maximal in the sense of containment. That is, for every k, for every query γ of semantic tree-width k and expansion k of semantic tree-width k there may be another expansion k such that k in fact, for classes of CRPQs avoiding such problematic behavior, Question 10.3 can be positively answered. We next show why.

Let us call a UC2RPQ *finitely-redundant* if there is no infinite chain $\xi_1(\bar{x}) \subsetneq \xi_2(\bar{x}) \subsetneq \cdots$ among its expansions. See Figure 17 for a non-example. Observe that the classes of CQs

¹⁶In reference to "promise constraint satisfaction problems" [BG21, Definition 2.3].

 $^{^{17}}$ By [CM13, Theorems 3.1 & 4.3], if the class has bounded semantic path-width, then the problem is in Path \subseteq paraNL; by [CM13, Theorems 3.1 & 5.5], if the class does not have bounded semantic path-width, then the problem is Tree-hard.

$$(i) \qquad b \qquad a^* \qquad a$$

$$(ii) \qquad b \qquad a^* \qquad a$$

$$(ii) \qquad b \qquad a^* \qquad a$$

FIGURE 17. (i) A simple non-finitely-redundant Boolean CRPQ. (ii) For every n, there is a homomorphism from the (n + 1)-expansion to the n-expansion, but no homomorphism in the converse direction.

and UCQs are finitely-redundant, and also the class of CRPQs with "no directed cycles", meaning no directed cycle in its underlying directed graph and no empty word ε in the atom languages.

Lemma 10.4. The class of CRPQs with no directed cycles is finitely-redundant.

Proof. By means of contradiction, let γ have no directed cycles and suppose there is an infinite chain $\xi_1(\bar{x}) \subsetneq \xi_2(\bar{x}) \subsetneq \cdots$ of expansions of γ . Hence, there must be an atom expansion which grows arbitrarily in the chain. Take ξ_i such that it contains an atom expansion of size bigger than ξ_1 . Since such atom expansion is a directed path (as we are dealing with one-way CRPQs), the fact that $\xi_i \xrightarrow{hom} \xi_1$ implies that there is some cycle in ξ_1 . Since γ cannot contain the empty word in the atom languages, this is in contradiction with the hypothesis that there are no directed cycles in γ .

We next show that, restricted to classes of finitely-redundant UC2RPQ, we can obtain a characterization of evaluation in FPT.

Theorem 10.5. Assuming W[1] \neq FPT, for any recursively enumerable class C of finitely-redundant Boolean UC2RPQs, the evaluation problem for C is FPT if, and only if, C has bounded semantic tree-width.

Proof. Left-to-right By contraposition, we show that if C has unbounded tree-width, then its evaluation problem is W[1]-hard via an FPT-reduction from the *parameterized clique* problem. This is the problem of, given a parameter k and a simple graph G, whether G contains a k-clique. We do this by a simple adaptation of the proof of Grohe [Gro07, Theorem 4.1] for the case of CQs.

Given an instance $\langle G, k \rangle$ of the parameterized clique problem, the idea is to first search for a query $\gamma \in C$ of "sufficiently large" semantic tree-width.

Let us call an expansion ξ of a UC2RPQ to be *maximal* if there is no other expansion ξ' such that $\xi \subsetneq \xi'$. The *core* of a CQ is the result of repeatedly removing any atom which results in an equivalent query. It is unique up to isomorphism (see, *e.g.*, [CM77]), and a CQ has semantic tree-width k iff its core has tree-width k [DKV02, Theorem 12]. We say that a CQ is 'a core' if it is isomorphic to its core.

Proposition 10.6. For any $k \ge 3$, if a finitely-redundant C2RPQ has semantic tree-width $\ge k$, then there is a maximal expansion thereof of semantic tree-width $\ge k$.

Proof. Let γ be a finitely-redundant C2RPQ. Consider the infinitary UCQ

 $\Xi = \{ \operatorname{core}(\xi) \mid \xi \text{ is a maximal expansion of } \gamma \}.$

Since γ is finitely-redundant, we have $\gamma \equiv \Xi$. We prove the fact by contraposition. If all maximal expansions of γ have semantic tree-width $\leq k-1$, then all CQs of Ξ have tree-width $\leq k-1$, and so by the implication $(1) \Rightarrow (3)$ of Theorem 3.13, query γ has semantic tree-width at most k-1. Note that for Theorem 3.13 to apply, we need k-1>1 i.e. $k \geq 3$.

Proposition 10.7. The set of all maximal expansions of queries from C is recursively enumerable.

Proof. We first show that given an expansion ξ of some C2RPQ γ , it is decidable whether ξ is maximal. This follows from the following claim: there exists an expansion ξ' of γ s.t. $\xi' \xrightarrow{hom} \xi$ and $\xi \xrightarrow{hom} \xi'$ iff there exists such an expansion whose atom expansions have length at most $2^m \cdot |\xi| \cdot |\mathbb{A}|^{2|\xi|}$ where $|\xi|$ is the number of variables of ξ and m is the greatest number of states of an NFA labelling an atom of γ . Decidability of maximality clearly follows from this claim: it suffices to check if $\xi' \xrightarrow{hom} \xi$ implies $\xi \xrightarrow{hom} \xi'$ for all "small" ξ' .

To prove the claim, let ξ' be an expansion of γ , and assume that there is a homomorphism $f \colon \xi' \to \xi$ and that $\xi \xrightarrow{hom} \xi'$. Consider an atom expansion

$$\pi' = x_0 \xrightarrow{a_1} x_1 \xrightarrow{a_2} \cdots \xrightarrow{a_{n-1}} x_{n-1} \xrightarrow{a_n} x_n$$

of ξ' , and let \mathcal{A} denote the NFA associated with the atom. For any index $i \in [0, n]$ which is neither among the $|\xi|$ first positions nor the $|\xi|$ last positions, define its type τ_i as the word $a_{i-|\xi|} - 1 \cdots a_i a_{i+1} \cdots a_{i+|\xi|}$ of length $2|\xi|$ —note that τ_i uniquely describes the ball of radius $|\xi|$ centred at x_i in ξ . Consider the function which maps index $i \in [|\xi|, n - |\xi| + 1]$ to the pair $\langle f(x_i), Q_i, \tau_i \rangle$, where Q_i is the set of states q of \mathcal{A} which admit a path from an initial state to q labelled by $a_1 \cdots a_i$. If $n \geq |\xi| \cdot 2^{|\mathcal{A}|} \cdot |A|^{2|\xi|} + 2|\xi|$ then by the pigeon-hole principle, there exists $i, j \in [|\xi|, n - |\xi| + 1]$ s.t. i < j, $f(x_i) = f(x_j)$, $Q_i = Q_j$ and $\tau_i = \tau_j$. Letting

$$\pi'' = x_0 \xrightarrow{a_1} x_1 \xrightarrow{a_2} \cdots \xrightarrow{a_{i-1}} x_{i-1} \xrightarrow{a_i} x_i = x_j \xrightarrow{a_{j+1}} x_{j+1} \xrightarrow{a_{j+2}} \cdots \xrightarrow{a_{n-1}} x_{n-1} \xrightarrow{a_n} x_n,$$

consider the query ξ'' obtained from ξ' by replacing π' with π'' . Since $Q_i = Q_j$, ξ'' is still an expansion of γ . Moreover, $f(x_i) = f(x_j)$ implies that there is a homomorphism from ξ'' to ξ . Lastly, it there was a homomorphism from ξ to ξ'' , then this homomorphism should contain x_i in its image—otherwise there would clearly be a homomorphism from ξ to ξ' . Note that the image of this homomorphism is included in the ball of ξ'' centered at $x_i = x_j$ of radius $|\xi|$. But since $\tau_i = \tau_j$ this ball is equal to the ball of ξ' centered at x_i (or equivalently at x_j) of radius $|\xi|$, and so we found a homomorphism from ξ to ξ' , which is not possible. Hence, there cannot be any homomorphism from ξ to ξ'' , which concludes the proof.

Finally, to enumerate all maximal expansions of queries from C, it suffices to enumerate all expansions of queries from C—which is doable since C is recursively enumerable—and only keep those which are maximal, using the previous algorithm.

We proceed with the reduction. For any value of k which is big enough, we enumerate all maximal expansions of C until we find one such expansion ξ whose core contains a $K \times K$ grid as a minor, for $K = \binom{k}{2}$. We know that this must happen by Proposition 10.6 and the Excluded Minor Theorem [RS86], stating that there exists a function $f: \mathbb{N} \to \mathbb{N}$ such that for every $n \in \mathbb{N}$ every graph of tree-width at least f(n) contains a $(n \times n)$ -grid as a minor. Once we get hold of such a maximal expansion ξ , we proceed as in [Gro07, proof of Theorem 4.1] to produce, in polynomial time, a graph database G_{ξ} such that:

- (1) there is a homomorphism $G_{\xi} \xrightarrow{hom} \xi$, and
- (2) G_{ξ} satisfies ξ if, and only if, G has a clique of size k.

Now consider the UC2RPQ $\Gamma \in \mathcal{C}$ of which ξ is an expansion, and observe that if G_{ξ} satisfies Γ , then we must have that G_{ξ} also satisfies ξ , by the fact that $G_{\xi} \xrightarrow{hom} \xi$ and ξ is maximal. Hence, the following are equivalent:

- G_{ξ} satisfies Γ ,
- G_{ξ} satisfies ξ ,
- G contains a k-clique.

This finishes the FPT-reduction.

Right-to-left This direction does not need any of the hypotheses (neither finite-redundancy, $W[1] \neq FPT$, nor r.e.), by Corollary 3.16.

10.3. Larger Classes. A natural and simple approach to extend the expressive power of CRPQs is to close the queries by transitive closure. That is, given a binary CRPQ $\gamma(x,y)$ we can consider CRPQ over the extended alphabet $\mathbb{A} \cup \{\gamma\}$, where the label γ is interpreted as the binary relation defined by $\gamma(x,y)$. This is the principle behind *Regular Queries* [RRV17]. The notion of tree-width can be easily lifted to this class, and classes of bounded tree-width still have a polynomial-time evaluation problem. However, this class has not yet been studied in the context of the semantic tree-width. It is not known if the semantic tree-width k problem is decidable, nor whether classes of bounded semantic tree-width have an FPT evaluation problem.

Question 10.8. Is the semantic tree-width k problem for Regular Queries decidable?

Query class	Membership problem	Evaluation problem
path-width $\leq k$ sem. path-w. $\leq k$	L-c [KM10, Theorem 1.3, p. 2] 2ExpSpace & ExpSpace-h (Theorem 8.7)	NL-c (Lemma 8.10) paraNL (Theorem 8.9)
tree-width $\leq k$ sem. tree-w. $\leq k$	L-c [EJT10, Lemma 1.4] 2ExpSpace & ExpSpace- h^{19} (Theorem 1.3)	P (Folklore) ¹⁸ FPT [RBV17, Corollary V.2] ²⁰ NP-c [RBV17, Theorem V.3]

TABLE 1. Complexity of the membership and evaluation problem for some classes of UC2RPQs studied in this paper, where $k \ge 1$ is fixed. The same results hold for the contracted variants. The abbreviation "-c" (resp. "-h") stands for "-complete" (resp. "-hard").

10.4. **Different Notions.** CRPQs of small tree-width or path-width enjoy a tractable evaluation problem, see Table 1. However, it must be noticed that containment between tree-width k or path-width k queries is still very hard: ExpSpace-complete (even for k = 1) [CDLV00]. The more restrictive measure of "bridge-width" [Fig20] has been proposed as

¹⁸Originally proven by Chekuri & Rajaraman [CR00, Theorem 3] for CQs. The generalization to UC2RPQs is trivial, see *e.q.* Proposition 1.1 or [RBV17, Theorem IV.3].

¹⁹See also [BRV16, Theorem 6.1] for k = 1.

²⁰See also Corollary 3.16 and [FGM24, Theorem 22].

a more robust measure, which results in classes of queries which are well-behaved both for evaluation (since bridge-width k implies tree-width $\leqslant k$) and for containment (since containment of bounded-bridge-width classes is in PSpace). It is not hard to see that bridge-width is closed under refinements, and thus that this notion is amenable to our approach (cf. Observation 3.5).

Question 10.9. Is the problem of whether a UC2RPQ is equivalent to a UC2RPQ of bridge-width at most k decidable?

APPENDIX A. POLYNOMIAL-TIME EVALUATION OF QUERIES OF BOUNDED TREE-WIDTH

Proposition 1.1. For each $k \ge 1$, the evaluation problem for UC2RPQs of tree-width at most k can be solved in time $\Theta(\|\Gamma\| \cdot |G|^{k+1} \cdot \log |G|)$ on a Turing machine, or $\Theta(\|\Gamma\| \cdot |G|^{k+1})$ under a RAM model, where Γ and G are the input UC2RPQ and graph database, respectively.

Proof. A semi-join is a CQ of the form $q(\bar{x}) = R(\bar{x}) \wedge S(\bar{y})$, noted $R(\bar{x}) \ltimes S(\bar{y})$, where \bar{x} and \bar{y} may contain common variables and constants. Yannakakis algorithm [Yan81] allows to evaluate any Boolean acyclic²¹ conjunctive query q on an n-tuple relational database in $\Theta(|q| \cdot c_{sj}(n))$, where $c_{sj}(n)$ is the cost of performing a semi-join: $\Theta(n \cdot \log(n))$ for Turing machines, or $\Theta(n)$ for a RAM model.²²

We reduce the evaluation problem for C2RPQs of tree-width k to the evaluation problem of Boolean acyclic CQs. First, if we receive $\Gamma(\bar{x})$, G and \bar{v} as input, we replace the free variables \bar{x} of Γ with the graph database nodes \bar{v} as constants, to obtain a Boolean C2RPQ (with constants). Let us therefore assume that Γ is Boolean. Take any $\gamma \in \Gamma$ and a tagged tree decomposition $(T, \mathbf{v}, \mathbf{t})$ of width at most k of γ .²³ It is easy to see that we can assume that the decomposition is of linear size in the number of atoms $\|\gamma\|_{\text{at}}$.²⁴ For every bag v of the decomposition containing $\mathbf{v}(v) = \{x_1, \dots, x_t\}$ consider the following relation R_v consisting of all tuples of database nodes (v_1, \dots, v_t) such that for every atom $A = x_i \xrightarrow{L} x_j$ in $\mathbf{t}^{-1}(v)$ we have that (v_i, v_j) satisfies A.

It then follows that

- (1) each R_v is of size $\mathcal{O}(|G|^{k+1})$,
- (2) the Boolean CQ $q = \bigwedge_{v \in V(T)} R_v(\mathbf{v}(v))$ is acyclic and of size linear in $\|\gamma\|_{\mathrm{at}}$, and
- (3) q is equivalent to γ .

Hence, Yannakakis algorithm yields a complexity of $\mathcal{O}(\|\gamma\| \cdot c_{sj}(|G|^{k+1}))$. That is, $\mathcal{O}(\|\gamma\| \cdot |G|^{k+1} \cdot \log |G|)$, or $\mathcal{O}(\|\gamma\| \cdot |G|^{k+1})$ in a RAM model.

We are only left with the cost of computing the relation R_v for any given $v \in V(T)$. Let $\mathcal{A}_v = \{A_1(y_1, z_1), \ldots, A_s(y_s, z_s)\}$ be the set of all atoms of $\mathbf{t}^{-1}(v)$. Let $\mathbf{v}(v) = \{x_1, \ldots, x_t\}$. Compute first the relation $S_i = \{(u, u') \in V(G)^2 : (u, u') \text{ satisfies } A_i(y_i, z_i)\}$ for every i; this can be done in $\mathcal{O}(|G| \cdot |L_i \times G^{\pm}|)$, where $L_i \times G^{\pm}$ is the product of the NFA for the regular language L_i of A_i and the expanded database G^{\pm} . Compute also the relation $U = V(G)^t$

²¹An *acyclic* CQ over arbitrary relational structures is one which admits a tree decomposition whose set of bags are the sets of variables of its atoms (also known as "generalized hyper tree-width 1" or " α -acyclicity" of its underlying hypergraph).

 $^{^{22}}$ We use Random Access Machines (RAMs) with domain \mathbb{N} , in which we assume that the RAM's memory is initialized to 0. For every fixed dimension $d \geq 1$ we have available an unbounded number of d-ary arrays A such that for given $(n_1, \ldots, n_d) \in \mathbb{N}^d$ the entry $A[n_1, \ldots, n_d]$ at position (n_1, \ldots, n_d) can be accessed in constant time. To compute $R(\bar{x}\,\bar{y}) \ltimes S(\bar{y}\,\bar{z})$, where \bar{y} are the only common variables between the atoms and n_R and n_S are the number of tuples in R and S respectively, we may assume that constants from the relations are encoded as numbers in binary, of size $\mathcal{O}(\log(n_R + n_S))$. We first encode the relation R projected onto \bar{y} , as an array A of the dimension of \bar{y} in $\mathcal{O}(n_R)$, by putting a '1' in A for each tuple of R. Then, for each tuple of S we test if the \bar{y} -projection belongs to A, if so we put a '2' in the array A, this is $\mathcal{O}(n_S)$. Finally, for each tuple of R we output the tuple if its projection onto \bar{y} has a '2' in A. This last step takes $\mathcal{O}(n_R)$.

²³By a tagged tree decomposition of γ we mean one for the identity $\gamma \xrightarrow{hom} \gamma$. The definition of tagged tree decompositions can be found in Section 4.

²⁴Indeed, observe that the decomposition resulting from contracting any edge so that one bag is contained or equal to the other is of linear size and preserves the width (see, e.g., [GLS02]).

²⁵That is, $L_i \times G^{\pm}$ is a database having pairs (q, v) where q is a state for the NFA \mathcal{A}_i of L_i and $v \in V(G^{\pm})$, and we have an edge $(q, v) \xrightarrow{a} (q', v')$ in $L_i \times G^{\pm}$ if $q \xrightarrow{a} q'$ and $v \xrightarrow{a} v'$ are in \mathcal{A}_i and G^{\pm} respectively.

in $\mathcal{O}(|G|^t)$ (hence in $\mathcal{O}(|G|^{k+1})$). Finally, we compute R_v by performing s nested semi-joins

$$((U(x_1,\ldots,x_t)) \ltimes S_1(y_1,z_1)) \ltimes S_2(y_2,z_2) \cdots) \ltimes S_s(y_s,z_s)$$

in $\mathcal{O}(s \cdot |G|^{k+1} \cdot c_{sj}(|G|^{k+1}))$, that is, in $\mathcal{O}(s \cdot |G|^{k+1} \cdot \log(|G|))$ or $\mathcal{O}(s \cdot |G|^{k+1})$ in a RAM model. Repeating this for every bag we can compute all the R_v 's in $\mathcal{O}(\|\gamma\| \cdot |G|^{k+1} \cdot \log(|G|))$ (observe that we iterate only once on each atom, since we are using a "tagged" decomposition) or $\mathcal{O}(\|\gamma\| \cdot |G|^{k+1})$ in a RAM model.

APPENDIX B. ALTERNATIVE UPPER BOUND FOR CONTAINMENT OF UC2RPQs

In Section 3, in order to prove the $2\mathsf{ExpSpace}$ upper bound to the semantic tree-width k problem (Lemma 3.10), we proved an upper bound on containment of UC2RPQs (Proposition 3.11) by relying on the notion of bridge-width. In this section, we give a slightly different bound, which is more elementary (in the sense that it does not rely on bridge-width) and still yields a $2\mathsf{ExpSpace}$ upper bound to the semantic tree-width k problem.

Proposition B.1. The containment problem $\Gamma \subseteq \Delta$ between two UC2RPQs can be solved in non-deterministic space $2^{c \cdot ||\Gamma||} + p_{\Delta} \cdot 2^{c \cdot m_{\Delta}}$, where m_{Δ} is the size of the greatest disjunct of Δ , namely $m_{\Delta} = \max\{||\delta_{\Delta}|| \mid \delta \in \Delta\}$, p_{Δ} is the number of disjuncts of Δ , and c is a constant.

Proof sketch. The proposition can be shown by close inspection of the standard containment problem for UC2RPQs [CDLV00, Theorem 5]: the containment problem is reduced, in this instance, to checking the inclusion between NFAs of the form²⁶

$$\mathcal{A}_{\Gamma} \subseteq^{?} \bigcup_{\delta \in \Lambda} \mathcal{A}_{\delta}, \tag{B.1}$$

where A_{Γ} is a regular expression which is exponential in $\|\Gamma\|$, and \mathcal{A}_{δ} has size exponential in $\|\delta\| \leq m_{\Delta}$. Should (B.1) not hold, there must exist a counterexample of size at most

$$2^{|\mathcal{A}_{\Gamma}|} \times \prod_{\delta \in \Delta} 2^{|\mathcal{A}_{\delta}|}$$

Letting p_{Δ} be the number of queries in Δ , we get that the logarithm of the expression above—representing the size of the non-deterministic space needed by the algorithm—is upper bounded by

$$c_0 \Big(|\mathcal{A}_{\Gamma}| + \sum_{\delta \in \Delta} |\mathcal{A}_{\delta}| \Big) \leqslant_{\text{eventually}} 2^{c \cdot ||\Gamma||} + p_{\Delta} \cdot 2^{c \cdot n_{\Delta}},$$

for some constants c_0 and c.

 $^{^{26}\}mathcal{A}_{\Gamma}$ and \mathcal{A}_{δ} are denoted A_1 and A_3 , respectively, in [CDLV00].

APPENDIX C. PATH-WIDTH IS NOT CLOSED UNDER REFINEMENTS

Fact 8.1. For each $k \ge 1$, the class of graphs of path-width at most k is not closed under expansions.

Proof. Let X be a set of k-1 variables. Consider the undirected multigraph G_k whose set of nodes is $X \cup \{y_0, y_1, y_2, y_3\}$ with the following edge set:

- each $X \cup \{y_i\}$ $(i \in \{0, 1, 2, 3\})$ is a clique,
- there is an edge from y_i to y_{i+1} for $i \in \{0, 1, 2\}$, and
- there is a second edge from y_1 to y_2 .

By definition, this graph has path-width exactly k: it is as least k since it contains a (k+1)-clique—namely $X \cup \{y_i, y_{i+1}\}$ —and, moreover the following sequence of bags—cf. Figure 15a—defines a path decomposition of G_k of width k:

$$\langle X \cup \{y_0, y_1\}, \ X \cup \{y_1, y_2\}, \ X \cup \{y_2, y_3\} \rangle.$$

Let \mathcal{G}'_k be the graph obtained by refining the second edge from y_1 to y_2 , into two edges $\langle y_1, z \rangle$ and $\langle z, y_2 \rangle$, where z is a new variable—see Figures 15b and 15d. We claim that \mathcal{G}'_k has path-width at least k+1. Indeed, let $\langle T, \mathbf{v}, \mathbf{t} \rangle$ be a path decomposition of \mathcal{G}'_k .

Note that $X \cup \{y_0, y_1\}$, $X \cup \{y_1, y_2\}$, $X \cup \{y_2, y_3\}$ and $\{z, y_1, y_2\}$ are cliques, so there must be bags of $\langle T, \mathbf{v}, \mathbf{t} \rangle$ containing each of them. Let $b_{0,1}$, $b_{1,2}$, $b_{2,3}$ and b_Z denote these bags—note that they do not have to be distinct.

- (1) If b_Z appears in T between at least two bags among $b_{0,1}$, $b_{1,2}$ and $b_{2,3}$ (as in Figure 15b), since $X \subseteq \mathbf{v}(b_{i,j})$ for all (i,j), then $X \subseteq \mathbf{v}(b_z)$. Hence $X \cup \{z,y_1,y_2\} \subseteq \mathbf{v}(b_z)$ and so b_z has k+2 elements.
- (2) Otherwise, w.l.o.g. b_z appears strictly before all three bags $b_{0,1}$, $b_{1,2}$ and $b_{2,3}$, as in Figure 15d. We consider the way $b_{0,1}$, $b_{1,2}$ and $b_{2,3}$ are ordered in the path decomposition. If $b_{0,1}$ or $b_{2,3}$ appears first, then they are located between b_z and $b_{1,2}$, which both contain $\{y_1, y_2\}$, and so this bag must also contain $\{y_1, y_2\}$, and so it has size at least k + 2. Otherwise, if $b_{1,2}$ appears first, depending on the relative ordering of $b_{0,1}$ and $b_{2,3}$, we either get that $y_2 \in \mathbf{v}(b_{0,1})$ or that $y_1 \in \mathbf{v}(b_{2,3})$. In both cases, we have a bag with at least k + 2 elements.

In all cases, the path decomposition has width at least k+1, showing that \mathcal{G}'_k has path-width at least 2^{27} k+1.

²⁷In fact it has path-width exactly k + 1.

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