Querying Graph Databases with XPath

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ABSTRACT

XPath plays a prominent role as an XML navigational language due to several factors, including its ability to express queries of interest, its close connection to yardstick database query languages (e.g., first-order logic), and the low complexity of query evaluation for many fragments. Another common database model — graph databases — also requires a heavy use of navigation in queries; yet it largely adopts a different approach to querying, relying on reachability patterns expressed with regular constraints.

Our goal here is to investigate the behavior and applicability of XPath-like languages for querying graph databases, concentrating on their expressiveness and complexity of query evaluation. We are particularly interested in a model of graph data that combines navigation through graphs with querying data held in the nodes, such as, for example, in a social network scenario. As navigational languages, we use analogs of core and regular XPath and augment them with various tests on data values. We relate these languages to first-order logic, its transitive closure extensions, and finite-variable fragments thereof, proving several capture results. In addition, we describe their relative expressive power. We then show that they behave very well computationally: they have a low-degree polynomial combined complexity, which becomes linear for several fragments. Furthermore, we introduce new types of tests for XPath languages that let them capture first-order logic with data comparisons and prove that the low complexity bounds continue to apply to such extended languages. Therefore, XPath-like languages seem to be very well-suited to query graphs.

Categories and Subject Descriptors

F.4.1 [**Mathematical logic and formal languages**]: Mathematical logic; H.2.3 [**Database management**]: Languages—*Query Languages*

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XPath, Graph Databases, data values

1. INTRODUCTION

Managing graph-structured data has been an active topic over the past few years; there are multiple existing systems, both proprietary and open-source, and there is a growing body of research literature on graph databases (see, e.g., a survey [5]). There are numerous uses in modern applications whose data structure is naturally represented as graphs: for instance, RDF triples are typically viewed as edges in labeled graphs [27, 33, 37] and so are connections between people in social networks [21, 39, 40]. The Semantic Web and social networks are often cited as the key application areas of graph databases, but there are many others such as biology, network traffic, crime detection, and modeling object-oriented data.

When it comes to querying graph databases, one can, of course, ask standard relational queries, for instance, about information on people in a social network. What makes graph databases different, however, is the ability to ask queries about their *topology*, essentially looking for reachability patterns and, more generally, subgraph patterns [11, 21, 20]. A basic building block for such queries is typically a *regular path query*, or an *RPQ*, that selects nodes connected by a path described by a regular language over the labeling alphabet [19]. Extensions of RPQs with more complex patterns, backward navigation, relations over paths, and mixing labels and data in nodes have been studied extensively too [1, 6, 7, 11, 12, 18, 32].

Over the past decade, navigational queries have been studied in depth in a different framework extending the relational model, namely in XML. Most formalisms for describing and querying XML crucially depend on its path language XPath [44]. The goal of XPath is seemingly very similar to the goal of many queries in graph databases: it describes properties of paths, taking into account both their purely navigational properties and data that is found in XML documents. The popularity of XPath is largely due to several factors:

- it defines many properties of paths that are relevant for navigational queries;
- it achieves expressiveness that relates naturally to yardstick languages for databases (such as first-order logic, its fragments, or extensions with some form of recursion); and
- it has good computational properties over XML, notably tractable combined complexity for many fragments and even linear-time complexity for some of them.

In view of these desirable properties, it is natural to ask whether XPath-like languages can achieve the right balance of expressiveness and complexity of query evaluation in the context of graph databases. This is the question we address in this paper.

There appear to be two ways to use XPath as a graph database language. The first possibility is to essentially stick to the idea of RPQs and use XPath to describe paths between nodes. While XPath on words with data is well understood by now [9, 22], this idea has a significant drawback: in the presence of data, evaluating RPQs quickly becomes intractable [32], ruling out XPath as an add-on to RPQs.

A different approach is to apply XPath queries to the entire graph database, rather than paths selected by RPQs and similar queries. This is the approach we pursue. To a limited extent it was tried before. On the practical side, XPath-like languages have been used to query graph data (e.g., [13, 26]), without any analysis of their expressiveness and complexity, however. On the theoretical side, several papers investigated XPath-like languages from the modal perspective, dropping the assumption that they are evaluated on trees, for instance, [2, 35]. In fact, this was mainly done in the context of semistructured data and preceded much of XPath investigation in the XML literature. The focus of papers such as [1, 2, 35] is primarily on static analysis (containment) and, in general, the settings disregard data values in graph databases.

Thus, our goal is to investigate how XPath-languages can be used to query graph databases. In particular, we want to understand both the navigational querying power of such languages, and their ability to handle navigation and data together in graph databases. In this investigation, we can take advantage of the vast existing XML literature on algorithmic and language-theoretic aspects of XPath.

Of course there is no such thing as *the* XPath: the language comes in many shapes and flavors. To start with, languages can talk about purely structural properties of documents, or they can add tests based on data values carried by documents. We have the same dichotomy for graph databases: in fact most earlier formalisms dealt with navigational queries [7, 11, 18, 19], but more recently extensions to data values have been looked at [20, 32].

The second key parameter is the expressiveness of navigational querying. The basic language one usually starts with is *core* XPath [16, 25]. It can also come in several versions, and what we use as the basic language here is essentially an adaption of Core XPath 2.0 [16] to graph databases. The reason behind it is the equivalence of the language to first-order logic, the yardstick language for relational databases (and we shall extend the equivalence to graph databases). For restricting expressiveness, we shall look at positive fragments (again, as is common in the XPath literature). For giving the language more power, we look at adding the transitive closure operator, obtaining an analog of *regular* XPath [12, 14, 16] which itself has close connections to PDL [28].

Flavor of the languages. We use several versions of XPath-like languages for graph databases. Like XPath (or closely related logics such as PDL and CTL*), they have node tests and path formulae, and as the basic axes they use letters from the alphabet labeling graph edges. For instance, $a^* \cdot (b^-)^*$ finds pairs of nodes connected by a path that starts with a-edges in the forward direction, followed by b-edges in the backward direction. The reader familiar with conjunctive RPQs will immediately recognize one in this expression, but the expressiveness of languages we consider is not limited to such queries. Formulae may include node tests: for instance, $a^*[c] \cdot (b^-)^*$ modifies the above expression by requiring that the node where the a-labels switch to b-labels also has an outgoing c-edge. And crucially, node tests can refer to data values and have XPath-like conditions over them. For instance, the expression $a^*[{=}5] \cdot (b^-)^*$ checks if the data value in that intermediate node is 5, and $a^*[\langle a = b \rangle] \cdot (b^-)^*$ checks if that node has two outgoing edges, labeled a and b, to nodes that store the same data value.

We define several versions of XPath for graph databases. The core language is denoted by $\mathsf{GXPath}_{\text{core}}$ and the analog of regular XPath by $\mathsf{GXPath}_{\text{reg}}$. We augment them by different types of tests on data values, such as testing for constant values (like $[{=}5]$), or for comparisons of data values at the end of paths (like $[\langle a = b \rangle]$).

Summary of the results. We start by studying the expressive power. The first set of results concerns with pure navigational power (no data-value comparisons). It turns out that $\mathsf{GXPath}_{\text{core}}$ captures precisely FO^3, first-order logic with 3 variables, like its analog (core XPath 2.0) on trees. The difference, though, is that on graphs $\text{FO} \neq \text{FO}^3$, but on trees the two are the same. The proof establishes connection with relation algebra [43] which was recently studied in connection with pure navigational querying of graph databases, but from a rather different angle (see [23, 24] which considered relative expressiveness of fragments of relation algebra based on sets of operators).

Note that on trees there is another way of capturing FO, by means of *conditional* XPath [36], which adds the until-operator. We show that on graphs the analog of conditional XPath goes beyond FO.

When we move to $\mathsf{GXPath}_{\text{reg}}$, we show that the positive fragment of it captures precisely the *nested regular expressions* [38], proposed as the navigational mechanism for SPARQL. This further confirms the usefulness of XPath for graph querying. Full $\mathsf{GXPath}_{\text{reg}}$ is more expressive and corresponds to a fragment of the transitive closure logic. We also show that it is incompatible with other graph languages

such as RPQs and several of their extensions.

With data value comparisons, we show that adding the two types of node tests described above increases expressiveness and we provide the exact comparisons of the power of language fragments with different types of tests. Even the strongest tests do not give $\mathsf{GXPath}_{\text{core}}$ the power to capture FO^3 with data value comparisons, but we produce a different type of tests that elevate the language to the full power of FO^3. These were introduced in [32]: an example of such a test is $a_=$, selecting a-labeled edges between nodes with the same value.

We then move to the study of the complexity of XPath languages. We further extend them with numerical path formulae: for instance, $a^{n,m}$, for $n < m$, says that two nodes are reachable by a path of as whose length is between n and m. These comparisons, proposed in the SPARQL recommendations [29], do not affect expressiveness, but they can make expressions much more succinct [33].

We show that the complexity of *all* XPath languages on graphs inherits nice properties from XPath on trees, due to the 'modal' nature of the language: the combined complexity is always polynomial. Even more, it is always a low-degree polynomial. In fact, the query complexity is linear for all the fragments we consider. The data complexity is not worse than quadratic for navigational $\mathsf{GXPath}_{\text{reg}}$ and linear for its positive fragments. With data comparisons added, data complexity becomes quadratic (or better) again. When numerical path formulae are added, the data complexity is not worse than cubic.

The main conclusion is that XPath-like languages over graph databases should not be overlooked due to the combination of their expressiveness and low complexity of query evaluation.

Remark. Many ideas behind XPath came from logics initially designed for arbitrary labeled transition systems, for instance PDL and CTL*. So, in a way, adapting XPath to graph databases, whose underlying model is, in essence, labeled transition systems, may look like going back to the origins. Nonetheless, this is not quite so, and there are indeed results to show that are specifically tailored to the graph database context.

To start with, we concentrate on graphs that carry *data*: this is crucial in the database scenario, but is generally disregarded in verification and model checking. Handling data has been studied extensively in the XPath context, so we can combine both model-checking techniques for navigational features with XPath techniques for handling data. Some of the features, such as counting, are specifically added in response to SPARQL recommendations.

The second distinction is that there is a mismatch between features naturally required by logics of programs and by logics for querying graph data. Even though an occasional fragment of an XPath-like language may coincide with an existing logic (e.g., PDL is what becomes navigational path-positive graph XPath in our classification), most of the time we concentrate on languages that do not have precise counterparts on the program logic side.

Organization. We define graph databases in Section 2. In Section 3 we introduce our XPath-like languages. In Section 4 we study their expressive power, and in Section 5 we investigate their complexity. In Section 6 we introduce new data tests that go beyond those present in XPath and study their expressiveness and complexity. Concluding remarks are in Section 7. Due to space limitations, most proofs are only sketched here.

2. PRELIMINARIES

We first describe graph databases. We assume a model in which edges are labeled by letters from a finite alphabet Σ and nodes can contain data values from a countably infinite set $\mathcal{D}$ (for instance, attributes of people in a social network). For simplicity of notation only, we assume a single data value per node, as is often done in modeling XML with data trees [42]. This is not a restriction at all, as different attributes can be added by adding extra outgoing edges with specified labels (again, in the same way as data trees model XML documents).

DEFINITION 2.1 (DATA GRAPHS). *A* data graph *(over Σ and $\mathcal{D}$) is a triple $G = \langle V, E, \rho\rangle$, where:*

- *V is a finite set of nodes;*
- *$E \subseteq V \times \Sigma \times V$ is a set of labeled edges; and*
- *$\rho : V \to \mathcal{D}$ is a function that assigns a data value to each node in V.*

When we deal with purely navigational queries, i.e., those not taking into account data values, we refer to graph $\langle V, E\rangle$, omitting the function ρ. We write E_a for the set of a-labeled edges, i.e., $E_a = \{(v, v') \mid (v, a, v') \in E\}$.

A path from node v_1 to v_n in a graph is a sequence

$$\pi = v_1 a_1 v_2 a_2 v_3 \dots v_{n-1} a_{n-1} v_n \tag{1}$$

such that each (v_i, a_i, v_{i+1}), for $i < n$, is an edge in E. We use the notation $\lambda(\pi)$ to denote the label of path π, i.e., the word $a_1 \dots a_{n-1} \in \Sigma^*$.

Navigation languages for graph databases.

Most navigational formalisms for querying graph databases are based on *regular path queries*, or *RPQ*s [19], and their extensions. An RPQ is an expression of the form $x \xrightarrow{L} y$, where L is a regular language over Σ (typically represented by a regular expression or an NFA). Given a Σ-labeled graph $G = \langle V, E\rangle$, the answer to an RPQ as above is the set of pairs of nodes (v, v') such that there is a path π from v to v' with $\lambda(\pi) \in L$.

Conjunctive RPQs, or *CRPQs* [18] are the closure of RPQs under conjunction and existential quantification. Formally,

they are expressions of the form

$$\varphi(\bar{x}) \;=\; \exists \bar{y} \bigwedge_{i=1}^{n} (z_i \xrightarrow{L_i} u_i), \tag{2}$$

where all variables z_i, u_i come from $\bar{x}, \bar{y}$. The semantics naturally extends the semantics of RPQs: $\varphi(\bar{a})$ is true in G iff there is a tuple $\bar{b}$ of nodes such that, for every $i \leq n$, every pair v_i, v_i' interpreting z_i and u_i is in the answer to the RPQ $z_i \xrightarrow{L_i} u_i$.

These have been further extended, for instance, to 2CRPQs that allow navigation in both directions (i.e., the edges can be traversed both forwards and backwards [11]), U2CRPQs that allow unions, or to *extended* CRPQs, in which paths witnessing the RPQs $z_i \xrightarrow{L_i} u_i$ can be named and compared for relationships between them, defined as regular or even rational relations [7, 6].

3. XPATH-LIKE LANGUAGES FOR GRAPHS

We follow the standard way of defining XPath fragments [10, 12, 22, 25, 36, 16] and introduce some variants of *graph XPath*, or GXPath, to be interpreted over graph databases. As usual, XPath formulae are divided into *path formulae*, producing sets of pairs of nodes, and *node tests*, producing sets of nodes. Path formulae will be denoted by letters from the beginning of the Greek alphabet ($\alpha, \beta, \ldots$) and node formulae by letters from the end of the Greek alphabet ($\varphi, \psi, \ldots$).

Since we deal with data values, we need to define *data tests* permitted in node formulae. There will be two kinds of them.

1. Constant tests: For each data value $c \in \mathcal{D}$, we have two tests $=c$ and $\neq c$. The intended meaning is to test if the data value in the current node equals to, or differs from, constant c.

   The fragment of GXPath that uses constant tests will be denoted by GXPath(c).

2. Equality/inequality tests: These are typical XPath (in)equality tests of the form $\langle \alpha = \beta \rangle$ and $\langle \alpha \neq \beta \rangle$, where α and β are path expressions. The intended meaning is to check for the existence of two paths, one satisfying α and the other satisfying β, which end with equal (resp., different) data values.

   The appropriate fragment will be denoted by GXPath(eq). If we have both constant tests and equality tests, we denote resulting fragments by GXPath(c, eq).

Next we define expressions of GXPath. As already mentioned in the introduction, we look at *core* and *regular* versions of XPath. They both have node and path expressions. Node expressions in all fragments are given by the grammar:

$$\varphi, \psi := \top \mid \mathsf{test} \;\mid\; \neg\varphi \;\mid\; \varphi \wedge \psi \;\mid \varphi \vee \psi \;\mid\; \langle \alpha \rangle$$

where test is one of the permitted data tests defined earlier, and α is a path expression.

The path formulae of the two flavors of GXPath are given below. In both cases a ranges over Σ.

Path expressions of *Regular graph XPath*, denoted by $\mathsf{GXPath}_{\text{reg}}$, are given by:

$$\alpha, \beta := \varepsilon \mid \_ \mid a \;\mid\; a^- \;\mid\; [\varphi] \;\mid\; \alpha \cdot \beta \;\mid\; \alpha \cup \beta \;\mid\; \overline{\alpha} \mid \alpha^*$$

Path expressions of *Core graph XPath* denoted by $\mathsf{GXPath}_{\text{core}}$ are given by:

$$\alpha, \beta := \varepsilon \mid \_ \mid a \;\mid\; a^- \;\mid\; a^* \;\mid\; a^{-*} \;\mid\; [\varphi] \;\mid\; \alpha \cdot \beta \;\mid\; \alpha \cup \beta \mid \overline{\alpha}$$

We call this fragment "Core graph XPath", since it is natural to view edge labels (and their reverse) in data graphs as the single-step axes of the usual XPath on trees. For instance, a and a^- could be similar to "child" and "parent". Thus, in our core fragment, we only allow transitive closure over navigational single-step axes, as is done in Core XPath on trees. Note that we did not explicitly define the counterpart of node label tests in GXPath node expressions to avoid notational clutter, but all the results remain true if we add them.

Finally, we consider another feature that was recently proposed in the context of navigational languages on graphs (such as in SPARQL 1.1 [29]), namely counters. The idea is to extend all grammars defining path formulae with new path expressions

$$\alpha^{n,m}$$

for $n, m \in \mathbb{N}$ and $n < m$. Informally, this means that we have a path that consists of some k chunks, each satisfying α, with $n \leq k \leq m$.

When counting is present in the language, we denote it by #GXPath, e.g., $\#\mathsf{GXPath}_{\text{core}}$.

Given these path and node formulae, we can combine $\mathsf{GXPath}_{\text{core}}$ and $\mathsf{GXPath}_{\text{reg}}$ with different flavors of node tests or counting, starting with purely navigational fragments (neither c nor eq tests are allowed) and up to having both c and eq tests. For example, $\#\mathsf{GXPath}_{\text{reg}}(\mathsf{c}, \mathsf{eq})$ is defined by mutual recursion as follows:

$$\alpha, \beta := \varepsilon \mid \_ \mid a \mid a^- \mid [\varphi] \mid \alpha \cdot \beta \mid \alpha \cup \beta \mid \overline{\alpha} \mid \alpha^* \mid \alpha^{n,m}$$
$$\varphi, \psi := \neg\varphi \mid \varphi \wedge \psi \mid \langle \alpha \rangle \mid =c \mid \neq c \mid \langle \alpha = \beta \rangle \mid \langle \alpha \neq \beta \rangle$$

with c ranging over constants.

We define the semantics with respect to a data graph $G = \langle V, E, \rho \rangle$. The semantics $[\![\alpha]\!]^G$ of a path expression α is a set of pairs of vertices and the semantics of a node test, $[\![\varphi]\!]^G$, is a set of vertices. The definitions are given in Figure 1. In that definition, by R^k we mean the k-fold composition of a binary relation R, i.e., $R \circ R \circ \ldots \circ R$, with R occurring k times.

Remark. Note that each path expression α can be transformed into a node test by the means of $\langle \alpha \rangle$ operator. In particular, we can test if a node has a b-successor by writing, for instance, $\langle b \rangle$. To reduce the clutter when using such tests in path expressions, we shall often omit the $\langle\rangle$ braces and write e.g. $a[b]$ instead of $a[\langle b \rangle]$.

Path expressions

$$
\begin{array}{rcl}
[\![\varepsilon]\!]^G & = & \{(v,v) \mid v \in V\} \\
[\![\_]\!]^G & = & \{(v,v') \mid (v,a,v') \in E \text{ for some } a\} \\
[\![a]\!]^G & = & \{(v,v') \mid (v,a,v') \in E\} \\
[\![a^-]\!]^G & = & \{(v,v') \mid (v',a,v) \in E\} \\
[\![\alpha^*]\!]^G & = & \text{the reflexive transitive closure of } [\![\alpha]\!]^G \\
[\![\alpha \cdot \beta]\!]^G & = & [\![\alpha]\!]^G \circ [\![\beta]\!]^G \\
[\![\alpha \cup \beta]\!]^G & = & [\![\alpha]\!]^G \cup [\![\beta]\!]^G \\
[\![\overline{\alpha}]\!]^G & = & V \times V - [\![\alpha]\!]^G \\
[\![[\varphi]]\!]^G & = & \{(v,v) \in G \mid v \in [\![\varphi]\!]^G\} \\
[\![\alpha^{n,m}]\!]^G & = & \bigcup_{k=n}^{m} ([\![\alpha]\!]^G)^k
\end{array}
$$

Node tests

$$
\begin{array}{rcl}
[\![\langle\alpha\rangle]\!]^G & = & \pi_1([\![\alpha]\!]^G) = \{v \mid \exists v' \ (v,v') \in [\![\alpha]\!]^G\} \\
[\![\neg\varphi]\!]^G & = & V - [\![\varphi]\!]^G \\
[\![\varphi \wedge \psi]\!]^G & = & [\![\varphi]\!]^G \cap [\![\psi]\!]^G \\
[\![\varphi \vee \psi]\!]^G & = & [\![\varphi]\!]^G \cup [\![\psi]\!]^G \\
[\![{=}c]\!]^G & = & \{v \in V \mid \rho(v) = c\} \\
[\![{\neq}c]\!]^G & = & \{v \in V \mid \rho(v) \neq c\} \\
[\![\langle\alpha = \beta\rangle]\!]^G & = & \{v \in V \mid \exists v', v'' \ (v,v') \in [\![\alpha]\!]^G, \ (v,v'') \in [\![\beta]\!]^G, \rho(v) = \rho(v')\} \\
[\![\langle\alpha \neq \beta\rangle]\!]^G & = & \{v \in V \mid \exists v', v'' \ (v,v') \in [\![\alpha]\!]^G, \ (v,v'') \in [\![\beta]\!]^G, \rho(v) \neq \rho(v')\}
\end{array}
$$

Figure 1: Semantics of Graph XPath expressions with respect to $G = \langle V, E, \rho\rangle$

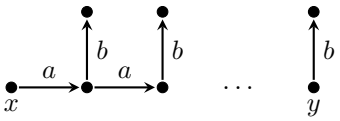
Basic expressiveness results.

Some expressions are readily definable with those we have. For instance, Boolean operations $\alpha \cap \beta$ and $\alpha - \beta$ with the natural semantics are definable. Indeed, $\alpha - \beta$ is definable as $\overline{\overline{\alpha} \cup \beta}$, and intersection is definable with union and complement. So when necessary, we shall use intersection and set difference in path expressions.

Counting expressions $\alpha^{n,m}$ are definable too: they abbreviate $\alpha \cdots \alpha \cdot (\alpha \cup \varepsilon) \cdots (\alpha \cup \varepsilon)$, where we have a concatenation of n times α and $m - n$ times $(\alpha \cup \varepsilon)$. Thus, adding counters does not influence expressivity of any of the fragments, since we always allow concatenation and union. However, counting expressions can be exponentially more succinct than their smallest equivalent regular expressions (independent of whether n and m are represented in binary or in unary) [33]. We will exhibit a query evaluation algorithm with polynomial-time complexity even for such expressions with counters represented in binary.

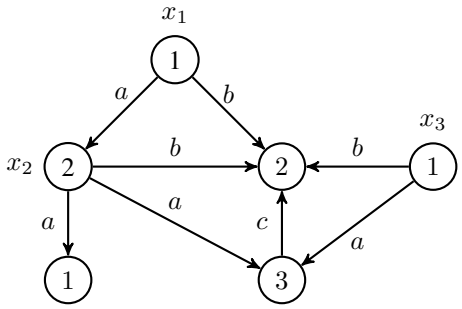
We next give three examples of GXPath expressions to illustrate what sort of queries one can ask using these languages.

1. The expression $(a[b])^*$ will simply give us all pairs (x, y) of nodes that are connected by a path of the following form:



   That is, x and y are connected by an a^* labelled path such that each node on the path also has an outgoing b-labelled edge. (Nodes that are different in the picture do not have to be different in the graph.)

2. The expression $\langle aa^* \neq bc^-\rangle$ will give us all nodes x such that there are nodes y and z, reachable by aa^* and bc^- respectively, with different data values. For example in the graph given in the following image the nodes x_1 and x_2 will be selected by our query, while x_3 will not.



3. The expression $\langle(a[{=}5] \cdot (a[{=}5])^*) \cap \varepsilon\rangle$ will extract all the nodes x such that there is a cycle starting at x in which each edge is labelled by a and each node has the data value 5. In particular the node x will have data value 5. Note that this example illustrates how we can define loops using GXPath.

As another observation on the expressiveness of the language, note that we can define a test $\langle\alpha = c\rangle$, with the semantics $\{v \mid \exists v' \ (v,v') \in [\![\alpha]\!]^G$ and $\rho(v') = c\}$, by using the expression $\langle\alpha[{=}c]\rangle$.

Another thing worth noting is that node expressions can be defined in terms of path operators. For example $\varphi \wedge \psi$ is defined by the expression $\langle\varepsilon[\varphi] \cdot \varepsilon[\psi]\rangle$, while $\neg\varphi$ is defined by $\langle\overline{\varepsilon[\varphi]}\rangle$.

Complement and positive fragments.

In standard XPath dialects on trees, complementation operators are not included and one usually shows that languages are closed under negation. This is no longer true for arbitrary graphs, due to the following.

PROPOSITION 3.1. *Neither $\overline{\alpha}$ nor $\alpha - \beta$ is definable in GXPath$_{reg}$ without complement on path expressions.*

The proof is an immediate consequence of the following observation. Given a data graph G, let $V_1, \ldots, V_m$ be sets of nodes of its (maximal) connected components (with respect to the edge relation $\bigcup_{a\in\Sigma} E_a$). Then a simple induction on the structure of the expressions of GXPath$_{\text{reg}}$ without complement on path expressions shows that for each expression α, we have $[\![\alpha]\!]^G \subseteq \bigcup_{i\leq m} V_i \times V_i$. However, both path complementation $\overline{\alpha}$ and path difference $\alpha - \beta$ violate this property.

In what follows, we consider fragments of our languages that restrict complementation and negation. There are two kinds of them, the first corresponding to the well-studied notion of positive XPath.

- The *positive fragments* are obtained by removing $\neg\varphi$ and $\overline{\alpha}$ from the definitions of node and path formulae. We use the superscript pos to denote them, i.e., we write GXPath$^{\text{pos}}_{\text{core}}$ and GXPath$^{\text{pos}}_{\text{reg}}$.
- The *path-positive fragments* are obtained by removing $\overline{\alpha}$ from the definitions of path formulae, but keeping $\neg\varphi$ in the definitions of node formulae. We use the superscript path-pos to denote them, i.e., we write GXPath$^{\text{path-pos}}_{\text{core}}$ and GXPath$^{\text{path-pos}}_{\text{reg}}$.

4. EXPRESSIVE POWER OF LANGUAGES

The goal of this section is to analyze the expressiveness of various XPath-like formalisms for graph databases that we introduced. We start with navigational features and then analyze languages that handle data comparisons. Additional analysis of expressiveness is given in Section 6 where we extend languages with more powerful comparisons of data.

4.1 Expressiveness of navigational languages

We provide three types of analysis of expressiveness of navigational features of dialects of graph XPath:

- We compare them with FO, fragments and extensions. The core language will capture FO^3. This is similar to a capture result for trees [36]; the main difference is that on graphs, unlike on trees, this falls short of full FO. We also provide a counterpart of this result for GXPath$_{\text{reg}}$, adding the transitive closure operator.
- We compare them with commonly used graph languages, such as nested regular expressions [38] and CRPQs (and relatives). We identify a fragment of GXPath$_{\text{reg}}$ that captures nested regular expressions, but show that generally, XPath flavors are incompatible with CRPQs and their extensions.
- We look at the analog of conditional XPath [36] which captures FO over trees and show that, in contrast, over graph databases, it can express queries that are not FO-definable.

4.1.1 Comparisons with FO and relatives

To compare expressiveness of GXPath fragments with first-order logic, we need to explain how to represent graph databases as FO structures. Since all the formalisms can express reachability queries (at least with respect to a single label), we view graphs as FO structures

$$G = \langle V, (E_a, E_{a^*})_{a\in\Sigma}\rangle$$

where $E_a = \{(v, v') \mid (v, a, v') \in E\}$ and E_{a^*} is its reflexive-transitive closure.

Recall that FO^k stands for the k-variable fragment of FO, i.e., the set of all FO formulae that use variables from a fixed set $x_1, \ldots, x_k$. As we mentioned, on trees, the core fragment of XPath 2.0 was shown to capture FO^3. We now prove that the same remains true without restriction to trees.

THEOREM 4.1. *GXPath$_{core}$ $= \text{FO}^3$ with respect to both path queries and node tests.*

Proof sketch. The idea behind this proof is to use the characterization of FO^3 in terms of relation algebras [43]. These are algebras of binary relations over some domain V and are closed under composition of relations, complementation (over V^2), union and reverse relation. We start with a base set $A_1, \ldots, A_n$ of binary relations over V and interpret the operations in a standard way. We shall be using relation algebras over V whose base relations are those in the FO vocabulary, i.e., the E_as and the E_{a^*}s.

We can then show that, for each FO^3 formula $F(x, y)$ with free variables x and y (in the vocabulary of the E_as and E_{a^*}s), there is a path expression α_F of GXPath$_{\text{core}}$ such that $(a, b) \in [\![\alpha_F]\!]^G$ iff $G \models F(a, b)$. This is done by going through relation algebra (with base binary relations E_a, E_{a^*}, for $a \in \Sigma$) and showing that such an algebra is equivalent with path expressions of GXPath$_{\text{core}}$ over the class of graphs where E_{a^*} is the reflexive transitive closure of E_a. The other direction is actually much simpler as we only have to give a translation from GXPath$_{\text{core}}$ formulas to FO^3 formulas.

Note that going through relation algebra works only for formulas with two free variables. To show that every formula $F(x)$ with a single free variable is equivalent to a GXPath$_{\text{core}}$ node test we can define $F'(x, y)$ as $(x = y) \wedge F(x)$, and find an equivalent path expression $\alpha_{F'}$. Then we simply set $\varphi_F := \langle\alpha_{F'}\rangle$ to get the node expression equivalent to F. □

Not all results about the expressiveness of XPath on trees extend to graphs. For instance, on trees, the regular fragment with no negation on paths (i.e., the path-positive fragment) can express all of FO [36]. This fails over graphs: GXPath$_{\text{reg}}$ fails to express even all of FO^2 when restricted to its path-positive fragment (i.e, the fragment that still permits unary negation).

PROPOSITION 4.2. *There exists a binary* FO^2 *query that is not definable in* $\mathsf{GXPath}_{reg}^{path\text{-}pos}$.

Proof sketch. The idea is to observe that path-positive fragments of GXPath cannot define the universal binary relation on an input graph. The query not definable in $\mathsf{GXPath}_{\mathrm{reg}}^{\mathrm{path\text{-}pos}}$ is then the one saying that there are at least two nodes in a given graph. □

We now move to $\mathsf{GXPath}_{\mathrm{reg}}$ and relate it to a fragment of FO^*, the parameter-free fragment of the transitive-closure logic. The language of FO^* extends the one of FO with a transitive closure operator that can be applied to formulas with precisely two free variables. That is, for any FO formula $F(x, y)$, the formula $F^*(x, y)$ is also an FO^* formula. The semantics is the reflexive-transitive closure of the semantics of F. That is, $G \models F^*(a, b)$ iff $a = b$ or there is a sequence of nodes $a = v_0, v_1, \ldots, v_n = b$ for $n > 0$ such that $G \models F(v_i, v_{i+1})$ whenever $0 \leq i < n$.

By $(\mathrm{FO}^*)^k$ we mean the k-variable fragment of FO^*. Note that when we deal with FO^* and $(\mathrm{FO}^*)^k$, we can view graphs as structures of the vocabulary $(E_a)_{a\in\Sigma}$, since all the E_{a^*}s are definable, and there is no reason to include them in the language explicitly.

Over trees, regular XPath is known to be equal to $(\mathrm{FO}^*)^3$ [14]. The next theorem shows that over graphs, these logics coincide as well.

THEOREM 4.3. $\mathsf{GXPath}_{reg} = (\mathrm{FO}^*)^3$.

Proof sketch. The containment of $\mathsf{GXPath}_{\mathrm{reg}}$ in $(\mathrm{FO}^*)^3$ is done by a routine translation.

To show the converse, we use techniques similar to those in the proof of Theorem 4.1: we extend $(\mathrm{FO}^*)^3$ and relation algebra equivalence to state that relation algebra with the transitive closure operator has equal expressive power to $(\mathrm{FO}^*)^3$ over the class of all labeled graphs. For this one can simply check that the inductive proof from [4] can be extended by adding two extra inductive clauses. Namely, when going from relation algebra to FO^3 we simply state that expressions of the form R^* are equivalent to $F_R^*(x, y)$, where F_R is the formula equivalent to R. In the other direction we simply state that $F^*(x, y)$ is equivalent to $(R_F(x, y))^*$. Here by $R_F(x, y)$ we denote the expression equivalent to $F(x, y)$, when the variables are used in that particular order. After that one verifies that the correctness proof of [4] applies. □

What about the relative expressive power of $\mathsf{GXPath}_{\mathrm{core}}$ and $\mathsf{GXPath}_{\mathrm{reg}}$? For positive fragments, known results on trees (see [16]) imply the following.

COROLLARY 4.4. $\mathsf{GXPath}_{core}^{pos} \subsetneq \mathsf{GXPath}_{reg}^{pos}$.

We shall later see that the strict separation applies to full languages. This is not completely straightforward even though $\mathsf{GXPath}_{\mathrm{core}}$ is equivalent to a fragment of FO, since the latter uses the vocabulary with transitive closures. This makes it harder to apply standard techniques, such as locality, directly. We shall see how to establish separation when we deal with conditional XPath in Section 4.1.3.

4.1.2 Comparisons with path queries

Our next goal is to compare the expressiveness of XPath formalisms for graphs with that of other established formalisms. We start with *nested regular expressions*, which have been proposed as a navigational mechanism of SPARQL for querying RDF data [38]. After that we look at traditional languages such as RPQs, CRPQs, and relatives.

Nested regular expressions. These expressions, abbreviated as NRE, over a finite alphabet Σ extend ordinary regular expressions with the nesting operator and inverses [38]. Formally they are defined as follows:

$$n := \varepsilon \mid a \mid a^- \mid n \cdot n \mid n^* \mid n + n \mid [n]$$

where a ranges over Σ.

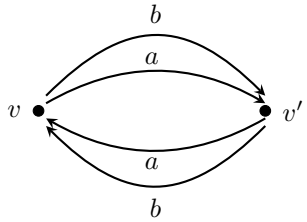
Intuitively NREs define binary relations consisting of pairs of nodes connected by a path specified by the NRE. When interpreted on a data graph G the relations are defined inductively as follows:

$$\begin{aligned}
[\![\varepsilon]\!]^G &= \{(v, v) \mid v \in V\} \\
[\![a]\!]^G &= \{(v, v') \mid (v, a, v') \in E\} \\
[\![a^-]\!]^G &= \{(v, v') \mid (v', a, v) \in E\} \\
[\![n \cdot n']\!]^G &= [\![n]\!]^G \circ [\![n']\!]^G \\
[\![n + n']\!]^G &= [\![n]\!]^G \cup [\![n']\!]^G \\
[\![n^*]\!]^G &= \text{the reflexive transitive closure of } [\![n]\!]^G \\
[\![[n]]\!]^G &= \{(v, v) \mid \exists v' \text{ such that } (v, v') \in [\![n]\!]^G\}.
\end{aligned}$$

As expected, $\mathsf{GXPath}_{\mathrm{reg}}$ is strictly more expressive than NREs. However, we show that NREs do capture the positive fragment of $\mathsf{GXPath}_{\mathrm{reg}}$.

THEOREM 4.5. $\mathsf{GXPath}_{reg}^{pos} = \mathsf{NRE} \subsetneq \mathsf{GXPath}_{reg}^{path\text{-}pos}$.

Proof sketch. To show that NREs are strictly weaker, consider a path formula $\alpha = a[\neg\langle b\rangle]$. Then one can prove by induction that over the graph below, every NRE has a nonempty answer.



This of course gives us the desired result, since $[\![\alpha]\!]^G = \emptyset$. □

Comparison with CRPQs. We will show that XPath-like formalisms are incomparable with CRPQs and similar queries in terms of their navigational expressiveness. The simple restriction, $\mathsf{GXPath}_{\mathrm{reg}}^{\mathrm{pos}}$, is not subsumed by

CRPQs. In fact it is not even subsumed by unions of two-way CRPQs (which allow navigation in both ways). On the other hand, CRPQs are not subsumed by the strongest of our navigational languages, $\mathsf{GXPath}_{\text{reg}}$.

THEOREM 4.6. *CRPQs and GXPath fragments are incomparable:*

- $\mathit{GXPath}^{pos}_{reg} \not\subseteq \mathit{CRPQ}$ *(even stronger, there are* $\mathit{GXPath}^{pos}_{reg}$ *queries not definable by U2CRPQs);*
- $\mathit{CRPQ} \not\subseteq \mathit{GXPath}_{reg}$.

Proof sketch. The first item follows from Theorem 4.5 and the fact that U2CRPQs cannot simulate certain NRE queries [8]. To see the second item, we first show that for every $\mathsf{GXPath}_{\text{reg}}$ expression e there exists an $\mathcal{L}^3_{\infty\omega}$ formula F_e equivalent to it. Recall that by $\mathcal{L}^3_{\infty\omega}$ we mean the infinitary first-order logic that uses only three variables (i.e. extension of FO^3 with infinite conjunctions and disjunctions). This is done by a standard induction on $\mathsf{GXPath}_{\text{reg}}$ expressions with variable reuse, see, e.g., [31].

Consider now two graphs, K_3 and K_4, with all edges labeled a. It is well know that they cannot be distinguished by $\mathcal{L}^3_{\infty\omega}$ since the duplicator has a winning strategy in the 3-pebble game on them. However, they can be distinguished by a CRPQ $\varphi(x, y)$ that states the existence of nodes z and u and all possible a-edges between x, y, z, u except self-loops. □

On the other hand, the positive fragment of $\mathsf{GXPath}_{\text{core}}$ can be captured by unions of two-way CRPQs.

PROPOSITION 4.7. $\mathit{GXPath}^{pos}_{core} \subsetneq \mathit{U2CRPQ}$.

4.1.3 *Conditional* GXPath

It was shown in [36] that to capture FO over XML trees, one can use *conditional* XPath, which essentially adds the temporal *until operator*. That is, it expands the core-XPath's a^* with $(a[\varphi])^*$, which checks that the test $[\varphi]$ is true on an a-labeled path. Formally, its path formulae are given by:

$$\alpha, \beta \quad := \quad \varepsilon \mid \_ \mid a \mid a^- \mid a^* \mid a^{-*} \mid (a[\varphi])^* \mid (a^-[\varphi])^* \mid [\varphi] \mid \alpha \cdot \beta \mid \alpha \cup \beta \mid \overline{\alpha}$$

We refer to this language as $\mathsf{GXPath}_{\text{cond}}$. We now show that the FO capture result fails rather dramatically over graphs: there are even positive $\mathsf{GXPath}_{\text{cond}}$ queries not expressible in FO.

THEOREM 4.8. *There is a* $\mathit{GXPath}^{pos}_{cond}$ *query not expressible in* FO.

Note that the standard inexpressibility tools for FO, such as locality, cannot be applied straightforwardly since the vocabulary of graphs already contains all the transitive closures E_{a^*}; in fact this means that in $\mathsf{GXPath}^{\text{pos}}_{\text{cond}}$ the query asking for transitive closures of base relations is trivially definable, even though it is not definable in FO over the E_as. So the way around this is to combine locality with the composition method: we use locality to establish a winning strategy for the duplicator in a game that does not involve transitive closures, and then use composition to extend the winning strategy to handle transitive closures.

Proof sketch. We consider graphs over alphabet $\{a, b, s, t\}$, with s, t being labels used to mark nodes between which we shall test reachability. We are interested in the following property P: from a node with an incoming s-edge to the node with an outgoing t-edge, there is an a-path such that each node on the path has a b-successor.

We then exhibit two families of graphs, G^m_1 and G^m_2, over the usual graph vocabulary, so that for each m we have $G^1_m \equiv_m G^2_m$ (i.e., the duplicator has a winning strategy in the usual m-round game), and all the G^1_ms have property P, and G^2_ms do not. To do so, we use Hanf-locality and the property that Hanf-locality, with a sufficiently long radius ($\geq 3^m$), implies the $\equiv_m$ relation (cf. [31]).

We then extend graphs G^m_1 and G^m_2 with a single new node v that has a-edges to and from every other node. Then a composition argument shows that the m-round winning strategy of the duplicator extends to the m-round winning strategy in the game on extended graphs viewed as structures in the vocabulary that includes all the transitive closures. Basically, the duplicator follows the original game on G^m_1 and G^m_2, and if the spoiler plays the new added node in one graph, then the duplicator responds with the added node in the other graph. What makes it work as a strategy in the extended vocabulary is that in the expanded graphs the interpretations of the transitive closures are easy: E_{a^*} is the total relation and no other relation E_x has a path of length 2. This implies that the property P is not FO-definable even in the expanded vocabulary.

But note that P is definable in $\mathsf{GXPath}_{\text{cond}}$ by $s(a[b])^*[t]$. So assuming $\mathsf{GXPath}_{\text{cond}} \subseteq \mathrm{FO}$ we get a contradiction. □

We can now fulfill our promise and establish separation between $\mathsf{GXPath}_{\text{core}}$ and $\mathsf{GXPath}_{\text{reg}}$. Since $\mathsf{GXPath}_{\text{core}} \subseteq \mathrm{FO}$ and we just saw a conditional (and thus regular) GXPath query not expressible in FO, we have:

COROLLARY 4.9. $\mathit{GXPath}_{core} \subsetneq \mathit{GXPath}_{reg}$.

4.2 Expressiveness of data languages

By coupling the basic navigational languages – $\mathsf{GXPath}_{\text{core}}$ and $\mathsf{GXPath}_{\text{reg}}$ – with various possibilities of data tests, such as no data tests, constant tests, equality tests, or both, we obtain eight languages, ranging from $\mathsf{GXPath}_{\text{core}}$ to $\mathsf{GXPath}_{\text{reg}}(\mathsf{c}, \mathsf{eq})$. Recall that adding counting does not affect expressiveness, only the complexity of query evaluation.

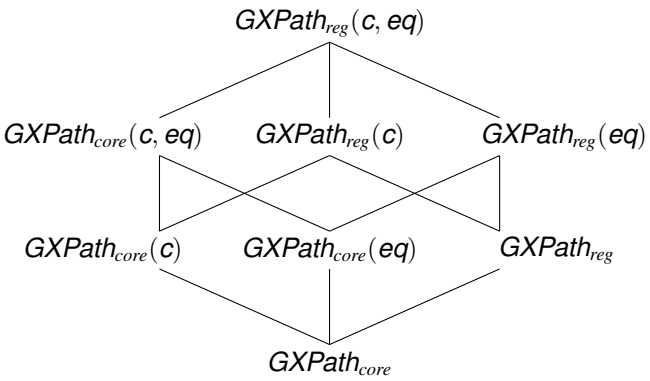
The question is then, how do these fragments compare to each other? Basically, each fragment is of the form $L(t)$, where L is the navigational language and t is the set of allowed data tests. We next show that there are no unexpected interdependencies: that is, $L(t)$ is strictly less expressive than $L'(t')$ iff:

1. $L \subseteq L'$ (in other words, $L = L'$ or $L = \mathsf{GXPath}_{\text{core}}$ and $L' = \mathsf{GXPath}_{\text{reg}}$),

2. $t \subseteq t'$; and
3. at least one of the above inclusions is strict (i.e., either $L = \mathsf{GXPath}_{\text{core}}$ and $L = \mathsf{GXPath}_{\text{reg}}$, or $t \subsetneq t'$).

Formally, we state the following.

THEOREM 4.10. *The relative expressive power of graph XPath languages with data comparisons is as shown below:*



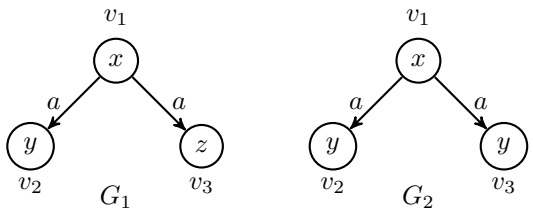
Here a line upwards means that the fragment is strictly contained in the other, while the lack of the line means that the fragments are incomparable.

Proof. The result follows from Corollary 4.9 (for navigational fragments) and the following two observations which show that c tests and eq tests are not mutually definable. Namely, take an alphabet Σ containing letter a. Let c be a fixed data value. Then:

- There is no $\mathsf{GXPath}_{\text{reg}}(\mathsf{eq})$ expression equivalent to the $\mathsf{GXPath}_{\text{core}}(\mathsf{c})$ query $q_{\mathsf{c}} := (= c)$.
- There is no $\mathsf{GXPath}_{\text{reg}}(\mathsf{c})$ expression equivalent to the $\mathsf{GXPath}_{\text{core}}(\mathsf{eq})$ query $q_{\mathsf{eq}} := \langle a = a \rangle$.

For the first item, simply take two single-node data graphs G_1 and G_2, with G_1's single node holding value c, and G_2 holding a different value c'. Hence, $[\![q_{\mathsf{c}}]\!]^{G_1}$ selects the only node of G_1, while $[\![q_{\mathsf{c}}]\!]^{G_2} = \emptyset$. However, a straightforward induction on the structure of expressions shows that for every $\mathsf{GXPath}_{\text{reg}}(\mathsf{eq})$ query e we have $[\![e]\!]^{G_1} = [\![e]\!]^{G_2}$.

For the second item assume that there is an $\mathsf{GXPath}_{\text{reg}}(\mathsf{c})$ expression ex equivalent to q_{eq}. Take any three pairwise distinct data values x, y, z that are different from all the constants appearing in ex and let G_1 and G_2 be as below:



One can show by straightforward induction on $\mathsf{GXPath}_{\text{reg}}(\mathsf{c})$ expressions e that use only constants appearing in ex that $[\![e]\!]^{G_1} = [\![e]\!]^{G_2}$. Thus, q_{eq} cannot be a $\mathsf{GXPath}_{\text{reg}}(\mathsf{c})$ expression, since $[\![q_{\mathsf{eq}}]\!]^{G_1} \neq [\![q_{\mathsf{eq}}]\!]^{G_2}$.

Note that this also shows that $\mathsf{GXPath}_{\text{core}} \subsetneq \mathsf{GXPath}_{\text{core}}(\mathsf{c})$ and $\mathsf{GXPath}_{\text{core}} \subsetneq \mathsf{GXPath}_{\text{core}}(\mathsf{eq})$. □

We saw that for navigational features, core graph XPath captures FO^3. The question is whether this continues to be so in the presence of data tests. First, we need to explain how to describe data graphs as FO-structures to talk about FO with data tests.

Following the standard approach for data words and data trees [42], we do so by adding a binary predicate for testing if two nodes hold the same data value. That is, a data graph is then viewed as a structure $G = \langle V, (E_a, E_{a^*})_{a \in \Sigma}, \sim \rangle$ where $v \sim v'$ iff $\rho(v) = \rho(v')$. To be clear that we deal with FO over that vocabulary, we shall write $\mathrm{FO}(\sim)$. If we want to talk about constant data tests (i.e., $=c$), we assume that the FO vocabulary contains constants. In that case we shall refer to $\mathrm{FO}(\mathsf{c}, \sim)$.

It turns out that the equivalence with FO^3 breaks when we add tests on data that have been seen so far.

THEOREM 4.11.
- $\mathsf{GXPath}_{\text{core}}(\mathsf{eq}) \subsetneq \mathrm{FO}^3(\sim)$;
- $\mathsf{GXPath}_{\text{core}}(\mathsf{c}, \mathsf{eq}) \subsetneq \mathrm{FO}^3(\mathsf{c}, \sim)$.

Proof sketch. The first containment uses the translation into FO^3 shown in the proof of Theorem 4.1. For the new data operators, we use the following. If $e = \langle \alpha = \beta \rangle$ then

$$F_e(x) \equiv \exists y, z(y \sim z \wedge F_\alpha(x, y) \wedge \exists y(z = y \wedge F_\beta(x, y)))$$

and likewise for the inequality comparison.

Translation of constants is self-evident.

To prove strictness we show that the FO^3 query $F(x, y) \equiv x \sim y$ is not definable in $\mathsf{GXPath}_{\text{reg}}(\mathsf{c}, \mathsf{eq})$. Note that F defines the set of all pairs of nodes carrying the same data value. The proof of this is implicit in the proof of Proposition 6.1. □

Thus, the standard XPath data tests are insufficient for capturing FO^3 over data graphs. Nonetheless, there is a simple extension of data tests that lets core graph XPath capture $\mathrm{FO}^3(\sim)$; we shall present it in Section 6.

5. COMPLEXITY OF QUERY EVALUATION

In this section we investigate the complexity of querying graph databases using variants of GXPath. We consider two problems. One is QUERY EVALUATION, which is essentially model checking: we have a graph database, a query (i.e., a path expression), and a pair of nodes, and we want to check if the pair of nodes is in the query result. That is, we deal with the following decision problem.

PROBLEM:	QUERY EVALUATION
INPUT:	A graph $G = (V, E)$, a path expression α, nodes $v, v' \in V$.
QUESTION:	Is $(v, v') \in [\![\alpha]\!]^G$?

The second version we consider is QUERY COMPUTATION, which actually computes the result of a query and outputs it. Normally, when one deals with path expressions, one fixes a context node v and looks for all nodes v' such that (v, v') satisfies the expression. We deal with a slightly more general version here, where the context node need not be single.

PROBLEM:	QUERY COMPUTATION
INPUT:	A graph $G = (V, E)$, a path expression α, and a set of nodes $S \subseteq V$.
OUTPUT:	All $v' \in V$ such that there exists a $v \in S$ with $(v, v') \in [\![\alpha]\!]^G$.

Note that in both problems we deal with *combined complexity*, as the query is a part of the input.

For measuring complexity, we let $|G|$ denote the size of the graph and $|\alpha|$ (resp., $|\varphi|$) denote the size of the path expression α (resp., node expression φ).

The main result of this section is that the combined complexity remains in polynomial time for all fragments we defined in Section 3. Not only that, but the exponents are low, ranging from linear to cubic. Notice that for navigational fragments, the low (and even linear) complexity should not come as a surprise. We noticed that $\mathsf{GXPath}_{\mathrm{reg}}^{\text{path-pos}}$ is essentially PDL, for which global model checking is known to have linear-time complexity [3, 17]. Also, polynomial-time combined complexity results are known for pure navigational $\mathsf{GXPath}_{\mathrm{reg}}$ from the PDL perspective as well [30].

Our main contribution is thus to establish the low combined complexity bounds for fragments that handle two new features we added on top of navigational languages: *data value comparisons* and *counters*. The former does increase expressiveness; the latter, as already remarked, does not, but it can make expressions exponentially more succinct. Thus, work is needed to keep combined complexity polynomial when counters are added.

For obtaining the linear-time complexities in this section, we assume a total order on the labels of edges. We assume that graphs are represented as adjacency lists such that we can obtain, for a given node v, the outgoing edges or the incoming edges, sorted in increasing order of labels, in constant time. (We note that the linear-time algorithm from [3] for PDL model checking also assumes that adjacency lists are sorted.) As we said, the following result is immediate from PDL model checking techniques:

FACT 5.1. *Both* QUERY EVALUATION *and* QUERY COMPUTATION *problems for* $\mathsf{GXPath}_{reg}^{path\text{-}pos}$ *can be solved in linear time, i.e.,* $O(|\alpha| \cdot |G|)$.

PROOF. Since global model checking for PDL is in linear time [3, 17], it is immediate that QUERY EVALUATION is in time $O(|\alpha| \cdot |G|)$. From this, the same bound for QUERY COMPUTATION can also be derived. Given a query α and a set S, we can mark the nodes in S with a special predicate that occurs nowhere in α. We can then modify query α and use the algorithm for global model checking for PDL to obtain the required output of QUERY COMPUTATION. □

The main upper bound in this section shows that combined complexity of both problems is polynomial for the most expressive language we have: regular graph XPath with counting, constant tests, and equality tests.

THEOREM 5.2. *Both* QUERY EVALUATION *and* QUERY COMPUTATION *problems for* $\#\mathsf{GXPath}_{reg}(\mathsf{c}, \mathsf{eq})$ *can be solved in polynomial time, specifically, i.e.,* $O(|\alpha| \cdot |G|^3)$.

Proof sketch. We can do a dynamic programming algorithm that considers the parse tree of α in a bottom-up fashion and computes, for every subexpression β of α, the table $[\![\beta]\!]^G$. For each subexpression φ, we store in a bit-vector the nodes of G that match φ.

When we see a subexpression of the form $\beta^{n,m}$, we compute the adjacency matrix representation of $[\![\beta]\!]^G$ and compute $[\![\beta^{n,m}]\!]^G$ by using fast squaring methods. This approach is similar to the one used for regular expressions with counters (cf. [33]). □

The algorithm for Theorem 5.2 is based on connectivity matrix multiplications for dealing with the counters. If the queries do not have counters, we can evaluate them more efficiently because we can avoid matrix multiplications. This allows us to drop data complexity from cubic to quadratic.

THEOREM 5.3. *Both* QUERY EVALUATION *and* QUERY COMPUTATION *problems for* $\mathsf{GXPath}_{reg}(\mathsf{c}, \mathsf{eq})$ *can be solved in polynomial time, specifically, i.e.,* $O(|\alpha| \cdot |G|^2)$.

The algorithm in the proof for Theorem 5.3 actually computes the entire relation $[\![\alpha]\!]^G$. Since the size of this relation can be quadratic in the worst-case, a significantly faster algorithm for computing $[\![\alpha]\!]^G$ cannot be expected.

A result related to Theorem 5.3 is shown in [30]. Here the combined complexity is investigated for an extension of PDL which includes the complement operator and context-free path expressions, and a model-checking algorithm based on adjacency matrix operation is presented. The algorithm from [30] uses time $O(|\varphi|^2 \cdot |V|^5)$, where $|V|$ is the number of nodes in G.

Finally, we give a fragment that takes data value comparisons into consideration and still permits linear-time query evaluation and computation. We do so by noticing that using only constant tests (as opposed to equality tests) does not introduce extra complexity for evaluation of path-positive GXPath. Since the latter is essentially PDL, we get an algorithm that is linear in both the query and the data. That is, we have the following.

THEOREM 5.4. *Both* QUERY EVALUATION *and* QUERY COMPUTATION *problems for* $\mathsf{GXPath}_{reg}^{path\text{-}pos}(\mathsf{c})$ *can be solved in linear time, i.e.,* $O(|\alpha| \cdot |G|)$.

6. BEYOND XPATH TESTS

We have seen previously that the equivalence of core graph XPath and FO^3 established for pure navigational fragments does not extend to data tests, as $\mathsf{GXPath}_{\text{core}}(\mathsf{eq}) \subsetneq \mathrm{FO}^3(\sim)$. This naturally leads to a question: what can be added to data tests to capture the full power of FO^3?

The answer to this is to add a different type of *equality comparison*, not present in XPath but used previously to enhance the power of RPQs and CRPQs [32]. These are defined by adding two expressions to the grammar for α: one is $\alpha_=$, the other is $\alpha_{\neq}$. Semantics, over data graphs, is

$$\begin{aligned} [\![\alpha_=]\!]^G &= \{(v,v') \in [\![\alpha]\!]^G \mid \rho(v) = \rho(v')\} \\ [\![\alpha_{\neq}]\!]^G &= \{(v,v') \in [\![\alpha]\!]^G \mid \rho(v) \neq \rho(v')\} \end{aligned}$$

In other words, we test whether data values at the beginning and at the end of a path are the same, or different. Such an extension is denoted by $\sim$, i.e. we talk about languages $\mathsf{GXPath}(\sim)$ (with the usual sub- and superscripts).

The first observation is that these tests indeed add to the expressiveness of the languages.

PROPOSITION 6.1. *The path query* $a_=$*, for* $a \in \Sigma$*, is not definable in* $\mathsf{GXPath}_{reg}(\mathsf{c}, \mathsf{eq})$.

Note that this query, $a_=$, is definable on trees by the $\mathsf{GXPath}_{\text{core}}(\mathsf{eq})$ query $[\langle \varepsilon = a \rangle] \cdot a \cdot [\langle \varepsilon = a^- \rangle]$. This is because the parent of a given node is unique. However, on graphs this is not always the case, and thus new equality tests add power.

The proof (omitted here) shows that, even though $\mathsf{GXPath}_{\text{reg}}(\mathsf{c}, \mathsf{eq})$ can test if a node has an a-successor with the same data value by the means of expression $\langle \varepsilon = a \rangle$, which will return the set $\{v \in V \mid \exists v' \in V \mid (v,v') \in [\![a_=]\!]^G\}$, it has no means of retrieving that specific successor.

With the extra power given to us by the equality tests, we can capture FO^3 over data graphs.

THEOREM 6.2. $\mathsf{GXPath}_{core}(\sim) = \mathrm{FO}^3(\sim)$.

Proof sketch. We follow the technique of the proof of Theorem 4.1. All of the translations used there still apply. The proof that relation algebra is contained in the language $\mathsf{GXPath}_{\text{core}}(\sim)$ is the same as without data values. We only have to add conversion of the new symbol $\sim$: if $R = \sim$, then $e = \varepsilon \cup (\bar{\varepsilon})_=$.

For the other direction we have to show how to translate new path expressions $\alpha_=$ and $\alpha_{\neq}$ into $\mathrm{FO}^3(\sim)$. This is done as follows: if $e = \alpha_=$ then $F_e(x,y) \equiv F_\alpha(x,y) \wedge x \sim y$ and likewise for inequality. The equivalences easily follow. Now the theorem follows from the equivalence of relation algebra and FO^3 [43]. □

From this we know that every $\mathsf{GXPath}_{\text{core}}(\mathsf{eq})$ query can be expressed in $\mathsf{GXPath}_{\text{core}}(\sim)$. We can also perform such a transformation explicitly. It is not difficult to see that every node expression of the form $\langle \alpha = \beta \rangle$ is equivalent to $\mathsf{GXPath}_{\text{core}}(\sim)$ expression $\langle \alpha \cdot (\alpha^- \cdot \beta)_= \cdot \beta^- \cap \varepsilon \rangle$, and similarly for $\neq$.

Query evaluation in the extended fragment.

We have added new features to the language. They increased its expressiveness, so the question arises whether the complexity of query evaluation (and query computation) suffers from this addition. The good news is that even with this addition, we retain polynomial combined complexity of both query evaluation and query computation, still with a low-degree polynomial.

THEOREM 6.3. *Both* QUERY EVALUATION *and* QUERY COMPUTATION *problems for* $\mathsf{GXPath}_{reg}(\mathsf{c}, \mathsf{eq}, \sim)$ *can be solved in polynomial time, specifically in time* $O(|\alpha| \cdot |G|^2)$.

Proof sketch. The algorithm is similar to the one of Theorem 5.3, which computes a table $[\![\beta]\!]^G$ for every path subexpression β. We now alter it so that, every time when we meet a subexpression of the form $\beta_=$, we walk through the table for $[\![\beta]\!]^G$ and remove all tuples with different data values, thus obtaining a table for $[\![\beta_=]\!]^G$. We proceed similarly for $[\![\beta_{\neq}]\!]^G$. □

7. CONCLUSIONS

After conducting the study of XPath-like languages over graph databases, our main conclusion is that they were perhaps unfairly overlooked as potential query languages. And indeed, some practitioners do attempt to use them [13, 26] probably following the intuition that such languages should behave well in the graph database context.

Our goal was to provide a theoretical foundation for this intuition. We did it by studying the expressiveness and complexity of various XPath formalisms over graph databases. Our languages included purely navigational features, to which one could add any of several features for handling data stored in graph databases. The navigational features corresponded to core and regular flavors of XPath, while data tests included different comparisons of data values: either XPath-like based on standard node tests, or more advanced, doing tests involving endpoints of paths.

We showed that the languages correspond to typical yardsticks for relational and XML languages. The navigational power of the core language captures FO^3, and this continues to be so with the most advanced data test (although typical XPath data tests fall short of the full FO power). For fragments based on regular XPath, we had correspondence with a three-variable fragment of the transitive closure logic.

We showed that the languages fit in well with some of the features proposed for SPARQL, the language for query-

ing RDF data. Specifically, we showed that one of the navigational fragments we deal with corresponds precisely to a popular navigational formalism for SPARQL, namely nested regular expressions, and we handled numerical tests on the numbers of repetitions of path, also proposed in the SPARQL standardization effort.

We then demonstrated that all the languages behave very well computationally: the combined complexity of all of them is polynomial. In fact, it is always a low-degree polynomial. The worst case complexity is cubic, and it applies only in the case of numerical tests, which are known to make expressions exponentially more succinct. In other cases, it is quadratic, and can even drop to linear for some fragments.

Given these desirable properties of XPath-like languages for graph databases, we believe this theoretical study justifies an attempt to experiment with those in practical scenarios, perhaps in less ad hoc way than was done in [13, 26]. As for a concrete language to adapt, we believe languages based on $\mathsf{GXPath}_{\mathrm{reg}}^{\text{path-pos}}$ hold a lot of promise. The navigational part is essentially PDL and therefore firmly rooted in logic. Complexity-wise it behaves like XPath: it can be evaluated in linear time and its satisfiability problem is EXPTIME-complete [28]. Perhaps more important, its proximity to XPath makes it very accessible to practitioners who are familiar with XML technology. In addition, as our study shows, it can be augmented with all other features (equality and constant tests, counting, even equality tests going beyond XPath) without incurring significant complexity costs.

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APPENDIX

Proofs

We note here that when dealing with expressivity results, we can assume that the wildcard _ is not present in the language, as it can be easily defined as $a_1 \cup \ldots \cup a_n$, where $\Sigma = \{a_1, \ldots, a_n\}$.

Proof of Theorem 4.1

To prove this we use a result of Tarski and Givant from [43] stating that relation algebra with the basis A of binary relations has the same expressive power as first order logic with three variables over the signature A of binary relations and equality.

As we will be using a slight modification of the result found in [43] we give precise formulation here. The proof of this version of the result can be found in [4] (see Theorem 1.9 and Theorem 1.10).

First we formalize relation algebras. Let $A = \{R_1, \ldots, R_n\}$ be a set of binary relation symbols. The syntax of relation algebra over A is defined as all expressions built from base relations in A using the operators $\cup, \overline{(\cdot)}, \circ, (\cdot)^-$, denoting union, complement, composition of relations and reverse relation. We are also allowed to use an atomic symbol Id denoting identity.

Our algebra is then interpreted over a structure $M = (V, R_1^M, \ldots, R_n^M)$ where all R_i^M are binary relations over V^2. Interpretations of symbols $\cup, \overline{(\cdot)}, \circ, (\cdot)^-$ and Id is the standard union, complement (with respect to V^2), composition and reverse of binary relations. Id is simply the set of all (v, v) where $v \in V$. We will write $(a, b) \in R^M$, or aR^Mb, when the pair (a, b) belongs to relation R defined over V with relations R_i interpreted as R_i^M.

THEOREM 8.1 ([4]). *Let $A = \{R_1, \ldots, R_n\}$ be a set of binary relation symbols.*

- *For every expression R in relation algebra $(A, \cup, \overline{(\cdot)}, \circ, (\cdot)^-, Id)$ there is an FO^3 formula in two free variables $\varphi_R(x, y)$, such that for every structure $M = (V, R_1^M, \ldots, R_n^M)$ we have*

$$\{(a, b) : aR^Mb\} = \{(a, b) : M \models \varphi_R[x/a, y/b]\}.$$

- *Conversely, for every FO^3 formula $\varphi(x, y)$, in two free variables, there exists a relation algebra expression R_φ such that for any structure $M = (V, R_1^M, \ldots, R_n^M)$ we have*

$$\{(a, b) : M \models \varphi[x/a, y/b]\} = \{(a, b) : aR_\varphi^Mb\}.$$

Note that we view a graph database $G = (V, E)$ as a structure over the alphabet of binary relations E_a, E_{a^*}, where $a \in \Sigma$. Then a graph database is interpreted as a model

$$M = (V, (E_a^M, E_{a^*}^M) : a \in \Sigma), \text{ where}$$

$$E_a = \{(v, v') : (v, a, v') \in E\}$$

and E_{a^*} is its reflexive transitive closure. Note that the Tarski-Givant result states something stronger, namely that the equivalence will hold over any structure, no matter if a^* is interpreted as the transitive closure of a or not. This means that it will in particular hold on all the structures where it is, and those are our graph databases.

First we give a translation from $\mathsf{GXPath}_{\text{core}}$ into FO^3. That is, for every path expression e, we provide a formula $F_e(x, y)$ in two free variables such that for, any graph database $G = (V, E)$, we have $[\![e]\!]^G = \{(v, v') \in G : M \models F_e[x/v, y/v']\}$, where $M = (V, (E_a^M, E_{a^*}^M) : a \in \Sigma)$ and $E_a = \{(v, v') : (v, a, v') \in E\}$ and E_{a^*} its reflexive transitive closure. Similarly, for every node expression φ, we define a formula $F_\varphi(x)$ in one free variable. The definition is by simultaneous induction on the structure of $\mathsf{GXPath}_{\text{core}}$ expressions.

Base cases:

- $e = a$ then $F_e(x, y) \equiv E_a(x, y)$
- $e = a^*$ then $F_e(x, y) \equiv E_{a^*}(x, y)$
- $e = a^-$ then $F_e(x, y) \equiv E_a(y, x)$

- $e = (a^-)^*$ then $F_e(x,y) \equiv E_a^*(y,x)$
- $\varphi = \top$ then $F_e(x) \equiv x = x$.

Inductive cases:

- $e = [\varphi]$ the $F_e(x,y) \equiv (x = y) \wedge F_{\varphi(x)}$
- $e = \alpha \cdot \beta$ then $F_e(x,y) \equiv \exists z(F_\alpha(x,z) \wedge \exists x(x = z \wedge F_\beta(x,y)))$
- $e = \alpha \cup \beta$ then $F_e(x,y) \equiv F_\alpha(x,y) \vee F_\beta(x,y)$
- $\varphi = \neg\psi$ then $F_\varphi(x) \equiv \neg F_\psi(x)$
- $\varphi = \psi \wedge \psi'$ then $F_\varphi(x) \equiv F_\psi(x) \wedge F_\psi(x)$
- $\varphi = \langle\alpha\rangle$ then $F_\varphi(x) \equiv \exists y F_\alpha(x,y)$
- $e = \overline{\alpha}$ then $F_e(x,y) \equiv \neg F_\alpha(x,y)$.

The claim easily follows. Note that we have shown that our expressions can be converted into FO^3 over a fixed interpretation of relation symbols appearing in our alphabet (that is when $E_{a^*} = (E_a)^*$). The result by Tarski and Givant is stronger, since it holds for any interpretation. Note that this does not invalidate our result, since we are interested only in this fixed interpretation of graph predicates.

To prove the equivalence of $\mathsf{GXPath}_{\text{core}}$ with FO^3 we now show that every relation algebra expression has an equivalent $\mathsf{GXPath}_{\text{core}}$ path expression.

First we show how to convert every relation algebra query into an equivalent $\mathsf{GXPath}_{\text{core}}$ expression over graph databases. To be more precise, we show that for any relation algebra expression R over the signature E_a, E_{a^*} there is a path expression e_R of $\mathsf{GXPath}_{\text{core}}$such that for any graph database $G = (V,E)$ it holds that $[\![e_R]\!]^G = \{(a,b) \in R^M\}$. Here M is obtained from G as before. In particular we assume that E_{a^*} is the reflexive transitive closure of E_a. We do this inductively on the structure of RA expressions R.

Base cases:

- If $R = E_a$ then $e = a$.
- If $R = E_{a^*}$ then $e = a^*$.
- If $R = Id$ then $e = \varepsilon$.

Inductive cases:

- If $R = R_1 \cup R_2$ then $e_R = e_{R_1} \cup e_{R_2}$.
- If $R = R_1 \circ R_2$ then $e_R = e_{R_1} \cdot e_{R_2}$.
- If $R = S^-$ then $e_R = (e_S)^-$.
- If $R = \overline{S}$ then $e_R = \overline{e_S}$.

To show the equivalence between $R = S^-$ and $e_R = (e_S)^-$ we need the following claim.

CLAIM 8.2. *For every GXPath_{core} path expression e there is a GXPath_{core} expression e^- such that $[\![e^-]\!]^G = \{(v,v') : (v',v) \in [\![e]\!]^G\}$, for every graph G.*

The proof of this is just an easy induction on expressions. We simply push the reverse onto atomic statements. Note that this is the reason why we can not simply drop the converse operators from our syntax.

All the other equivalences follow from the definition and the inductive hypothesis.

Now let $\varphi(x,y)$ be an arbitrary FO^3 formula. By Theorem 8.1 we know that there is a relation algebra expression R_φ equivalent to φ over all structures that interpret $\{E_a, E_{a^*} : a \in \Sigma\}$. In particular it is true over all the structures where $E_{a^*} = (E_a)^*$. By the previous paragraph we know that there is a $\mathsf{GXPath}_{\text{core}}$ expression e_{R_φ} equivalent to R_φ.

In particular this means that for every graph database $G = (V,E)$ it holds that for the model $M = (V, (E_a, E_{a^*}) : a \in \Sigma)$, derived from G, we have the following:

$$\{(a,b) : M \models \varphi[x/a, y/b]\} = \{(a,b) : (a,b) \in R_\varphi^M\}.$$

On the other hand, we also have:

$$[\![e_{R_\varphi}]\!]^G = \{(a,b) : (a,b) \in R_\varphi^M\}.$$

Thus we conclude that

$$\{(a,b) : M \models \varphi[x/a, y/b]\} = [\![e_{R_\varphi}]\!]^M.$$

The previous part shows equivalence between path expressions and formulas with two free variables. To deal with formulas with a single free variable $F(x)$ we do the following. Define $F'(x,y) = x = y \wedge F(x)$. Note that F' selects all pairs (v,v) such that $F(v)$ holds. Now find an equivalent path expression α (we know we can do this by going through relation algebra) and let $\varphi = \langle\alpha\rangle$.

Proof of Proposition 4.2

Let $\psi(x,y) \equiv \exists x \exists y(\neg x = y)$. It is easy to see that $[\![\psi]\!]^G = \{(x,y) : (x,y) \in V^2\}$ if $G = \langle V, E\rangle$ has at least two nodes and $[\![\psi]\!]^G = \emptyset$ otherwise. (Notice that the variables x, y in ψ are immediately "overwritten" by the existential quantification.)

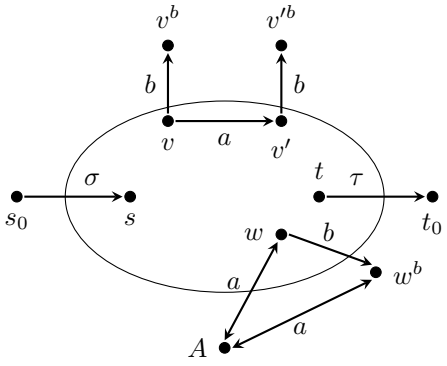
Consider the graphs $G_1 = \langle\{v, v'\}, \emptyset\rangle$ and $G_2 = \langle\{v\}, \emptyset\rangle$. That is, we have no edges. It follows that $[\![\psi]\!]^{G_1} = \{(v,v'), (v',v)\}$ and $[\![\psi]\!]^{G_2} = \emptyset$. It can be shown by induction on the structure of path $\mathsf{GXPath}_{\text{reg}}^{\text{path-pos}}$ expressions that we either have that $[\![\alpha]\!]^{G_1} = \{(v,v),(v',v')\}$ and $[\![\alpha]\!]^{G_2} = \{(v,v)\}$, or $[\![\alpha]\!]^{G_1} = \emptyset$ and $[\![\alpha]\!]^{G_2} = \emptyset$. Similarly for node expressions it can be shown that either $[\![\varphi]\!]^{G_1} = G_1$ and $[\![\varphi]\!]^{G_2} = G_2$, or $[\![\varphi]\!]^{G_1} = \emptyset$ and $[\![\varphi]\!]^{G_2} = \emptyset$.

Proof of Theorem 4.8

To prove this we will need several auxiliary results.

Let $\Sigma = \{a, b, \sigma, \tau\}$ be an alphabet of labels. We define a class $\mathcal{C}$ of Σ-labeled graphs as follows.

Take any graph $G = (V, E)$ over the singleton alphabet $\{a\}$ of labels. Fix two nodes s and t in G. Let $G^{\mathcal{C}}(s,t)$ be the graph obtained from G as follows. First, it contains all the nodes and edges of G. For every node $v \neq s, t$ in G we add a new node v^b and an edge edges (v, b, v^b) to $G^{\mathcal{C}}(s,t)$. We also add two new nodes, s_0 and t_0, together with edges (s_0, σ, s) and (t, τ, t_0), coming into s and leaving t. These nodes and edges are added to distinguish s and t in our graph. Finally, we add one extra node called A, and for every other node in $G^{\mathcal{C}}(s,t)$ we add two edges, one going into A and the other returning from A to the same node, both labeled a. Now add this $G^{\mathcal{C}}(s,t)$ to $\mathcal{C}$. The modifications are illustrated in the following image.



Also define $\mathcal{C}^-$ to be the class of graphs that are obtained from the graphs in $\mathcal{C}$ by removing the node A and all the associated edges.

Now let the property P stand for

- t is reachable from s via a path labeled with $(a[b])^*$.

That is, t is reachable from s by a path that proceeds forwards by a-labeled edges, but also has to have a b labeled edge leaving every internal node on the path.

To obtain the desired result we will first prove the following claim.

CLAIM 8.3. *The property P is not expressible in* FO *in vocabulary $\{E_a, E_b, E_\sigma, E_\tau, E_{a^*}, E_{b^*}, E_{\sigma^*}, E_{\tau^*}\}$ over the class $\mathcal{C}$. Here, as before, we assume that E_{ℓ^*} is the reflexive transitive closure of E_ℓ, for $\ell \in \{a, b, \sigma, \tau\}$.*

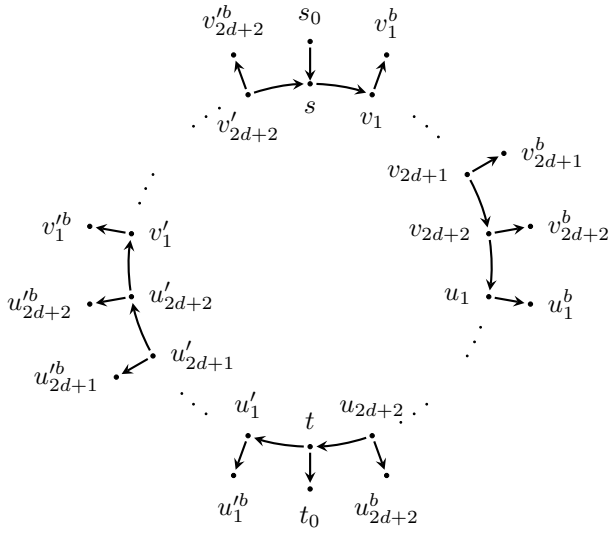
To prove this claim we will use Hanf-locality and composition of games. For the proof we use three lemmas.

In the first one, we use the standard notion of a *neighborhood* of an element in a structure, and the notion of Hanf-locality. For details, see [31]. Specifically, for two graphs G^1, G^2, we write $G^1 \leftrightarrows_d G^2$ if there is a bijection f between nodes of G^1 and nodes of G^2 (in particular, the sets of nodes must have the same cardinality) such that the radius-d neighborhoods of each node v in G^1 and $f(v)$ in G^2 are isomorphic. The radius-d neighborhood around v is the substructure generated by all nodes reachable from v by a path (using all types of edges) of length at most d.

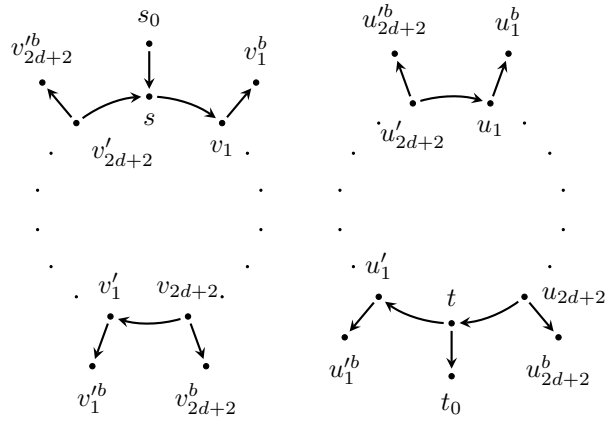
Locality is meaningless over structures in $\mathcal{C}$, since every two nodes are connected by a path of length 2, so $\leftrightarrows_2$ is isomorphism. This is why we get the result in several steps.

LEMMA 8.4. *For every $d \geq 0$ there exist two graphs G^1_d and G^2_d, as structures of the vocabulary $\{E_a, E_b, E_\sigma, E_\tau\}$, in $\mathcal{C}^-$ such that $G^1_d \leftrightarrows_d G^2_d$ and G^1_d satisfies P, while G^2_d does not.*

PROOF. To see this take arbitrary d and let the graphs G^1_d and G^2_d be as in the following two images. All the labels on the circles are a, the incoming edges from s_0's to the s's are labeled σ, the outgoing edges from the t's to t_0's are labeled τ, and the edges from the v's to the v^b's are labeled b.



Graph G^1_d



Graph G^2_d

Now let $f : G^1_d \to G^2_d$ be the bijection defined by the node labels in the natural way: each node gets mapped to the one with the same name in the other graph. That is we set $f(s) := s, f(v_i) := v_i$, then $f(v^b_i) := v^b_i$ and similarly for v'_i, u_i, etc.

To see that $G^1_d \leftrightarrows_d G^2_d$ we have to check $N^{G^1_d}_d(c) \cong N^{G^2_d}_d(f(c))$ for every c. But this is now easily established, since the d neighborhood of any c and $f(c)$ will simply be extended chains of length d around c and $f(c)$. In particular, it is possible that they intersect the d neighborhood of either s or t, but never both. We thus conclude that they will always be isomorphic, giving us the desired result. $\square$

Now from Lemma 8.4 and Corollary 4.21 in [31], which shows that Hanf-locality with a sufficiently large radius implies the winning strategy for the duplicator in an Ehrenfeucht-Fraïssé game, we obtain the following.

LEMMA 8.5. *For every $m \geq 0$ there exists $d \geq 0$ so that $G^1_d \equiv_m G^2_d$.*

As usual, by $\equiv_m$ we denote the fact that duplicator has a winning strategy in an m-round Ehrenfeucht-Fraïssé game. This game is still played on structures in the vocabulary that does not use transitive closures.

Now let $\mathbf{G}^1_d$ and $\mathbf{G}^2_d$ be obtained from G^1_d and G^2_d by adding, as in the picture above, a node A with a-edges to and from every other node. We view these graphs as structures of the vocabulary that has all the relations E_ℓ and E_{ℓ^*} for each of the four labels ℓ we have. Next, we show

LEMMA 8.6. *If $G^1_d \equiv_m G^2_d$, then $\mathbf{G}^1_d \equiv_m \mathbf{G}^2_d$.*

The strategy is very simple: the duplicator plays by copying the moves from the game $G^1_d \equiv_m G^2_d$ as long as the spoiler does not play the A-node. If the spoiler plays the A-node in one structure, the duplicator responds with the A-node in the other. We now need to show that this preserves all the relations. Clearly this strategy preserves all the relations E_ℓ among nodes other than the A-node, simply by assumption. Moreover, since $E_{\ell^*} = E_\ell$ for $\ell \neq a$, we have preservation of the transitive closures other than that of E_a as well. So we need to prove that the strategy preserves E_{a^*}, but this is immediate since in both graphs E_{a^*} is interpreted as the total relation. This proves the lemma.

The claim now follows from the lemmas: assume that P is expressible in FO, over the full vocabulary, by a formula of quantifier rank m. Pick sufficiently large d to ensure that $\mathbf{G}^1_d \equiv_m \mathbf{G}^2_d$. Then $\mathbf{G}^1_d$ and $\mathbf{G}^2_d$ must agree on P, but they clearly do not, since the extra paths introduced in these graphs compared to G^1_d and G^2_d go via the A-node, which does not have a b-successor.

Now to prove Theorem 4.8 consider a conditional graph XPath expression $\sigma(a[b])^*[\tau]$. Over graphs as considered here it defines precisely the property P, which, as just shown, is not FO-expressible in the full vocabulary.

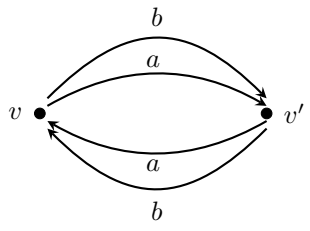
Proof of Theorem 4.5

First we show that $\mathsf{NRE} \subsetneq \mathsf{GXPath}_{\text{reg}}$.

It is a straightforward inductive construction that shows us how to convert nested regular expressions into an equivalent path expression of $\mathsf{GXPath}_{\text{reg}}$. Note that all the operations can be written down verbatim, minus the $[n]$ expression whose $\mathsf{GXPath}_{\text{reg}}$ equivalent is $[\langle e_n \rangle]$, where e_n is an expression equivalent to n.

Next we show that $\mathsf{GXPath}_{\text{core}}$ query $q = a[\neg\langle b \rangle]$ is not expressible by any NRE.

Consider the following data graph G.



It is easy to see that $[\![q]\!]^G = \emptyset$. We now show that $[\![n]\!]^G \neq \emptyset$, for any nested regular expression n. Thus we conclude that no equivalent NRE exists.

In fact we show that for every NRE n there exist nodes $x_1, x_2, y_1, y_2 \in \{v, v'\}$ such that $(v, x_1), (v', x_2), (y_1, v), (y_2, v') \in [\![n]\!]^G$.

This can be shown by an easy induction on the structure of n.

We now show that $\mathsf{GXPath}_{\text{reg}}^{\text{path-pos}} = \mathsf{NRE}$.

We already know that nested regular expressions can be expressed as GXPath queries. Examining the proof shows us that no negation is needed for this.

Next we show how to convert any $\mathsf{GXPath}_{\text{reg}}^{\text{pos}}$ expression into an equivalent nested regular expression. More precisely, we show that for any path expression α of our fragment there exists a nested regular expression n_α such that for any graph G we have $(x, y) \in [\![\alpha]\!]^G$ iff $(x, y) \in [\![n_\alpha]\!]^G$. Moreover, for any node expression φ we define a nested regular expression n_φ such that $x \in [\![\varphi]\!]^G$ iff $(x, x) \in [\![n_\varphi]\!]^G$. We do this by induction on the structure of our $\mathsf{GXPath}_{\text{reg}}^{\text{pos}}$ expressions.

Basis:

- $e = a$ then $n_e = a$
- $e = a^-$ then $n_e = a^-$
- $e = \varepsilon$ then $n_e = \varepsilon$
- $e = \top$ then $n_e = \varepsilon$

Inductive step:

- $e = [\varphi]$ then $n_e = [n_\varphi]$
- $e = \alpha \cdot \beta$ then $n_e = n_\alpha \cdot n_\beta$
- $e = \alpha \cup \beta$ then $n_e = n_\alpha + n_\beta$
- $e = \varphi \wedge \psi$ then $n_e = \varepsilon[n_\varphi] \cdot \varepsilon[n_\psi]$
- $e = \varphi \vee \psi$ then $n_e = \varepsilon[n_\varphi + n_\psi]$
- $e = \langle\alpha\rangle$ then $n_e = \varepsilon[n_\alpha]$.

It is easy to see the equivalence between defined expressions.

Proof of Theorem 4.6

Note that the first item follows from Theorem 4.5 and Theorem 1 in [8].

To see that the second item holds we first show that for every $\mathsf{GXPath}_{\text{reg}}$ expression e there exists an $\mathcal{L}^3_{\infty\omega}$ formula F_e equivalent to it. After that we give an example of a CRPQ that is not expressible in this logic using a standard multi-pebble games argument.

To be more precise we will be working with $\mathcal{L}^3_{\infty\omega}$ formulas over the alphabet $\{E_a : a \in \Sigma\}$ (and with the equality symbol). All the relations are binary and simply represent a labeled edge between two nodes. We will denote data graphs as structures for this logic by $G = \langle V, (E_a)_{a\in A}, =\rangle$.

Now for every path expression α we will define a formula $F_\alpha(x, y)$ such that $(v, v') \in [\![\alpha]\!]^G$ iff $G \models F_\alpha[x/v, y/v']$. Likewise for a node expression φ we define a formula $F_\varphi(x)$ such that $v \in [\![\varphi]\!]^G$ iff $G \models F_\varphi[x/v]$.

We do this by induction on $\mathsf{GXPath}_{\text{reg}}$ expressions.

Basis:

- $\alpha = a$ then $F_\alpha(x, y) \equiv E_a(x, y)$
- $\alpha = a^-$ then $F_\alpha(x, y) \equiv E_a(y, x)$
- $\alpha = \varepsilon$ then $F_\alpha(x, y) \equiv x = y$
- $\varphi = \top$ then $F_\alpha(x) \equiv x = x$

Inductive step:

- $\alpha' = [\varphi]$ then $F_{\alpha'}(x, y) \equiv x = y \wedge F_\varphi(x)$
- $\alpha' = \alpha \cdot \beta$ then $F_{\alpha'}(x, y) \equiv \exists z(\exists y\ (y = z \wedge F_\alpha(x, y)) \wedge \exists x\ (x = z \wedge F_\beta(x, y)))$
- $\alpha' = \alpha \cup \beta$ then $F_{\alpha'}(x, y) \equiv F_\alpha(x, y) \vee F_\beta(x, y)$
- $\alpha' = \alpha^*$ then define
  - $\varphi^1_\alpha(x, y) \equiv F_\alpha(x, y)$,
  - $\varphi^{n+1}_\alpha(x, y) \equiv \exists z\ (\exists y\ (y = z \wedge F_\alpha(x, y)) \wedge \exists x\ (x = z \wedge \varphi^n_\alpha(x, y)))$

  - Finally, set $F_{\alpha'}(x,y) \equiv \bigvee_{n\in\omega} \varphi^n_\alpha(x,y)$
- $\alpha' = \overline{\alpha}$ then $F_{\alpha'}(x,y) \equiv \neg F_\alpha(x,y)$
- $\varphi' = \neg\varphi$ then $F_{\varphi'}(x) \equiv \neg F_\varphi(x)$
- $\varphi' = \varphi \wedge \varphi$ then $F_{\varphi'}(x) \equiv F_\varphi(x) \wedge F_\psi(x)$
- $\varphi' = \langle\alpha\rangle$ then $F_{\varphi'}(x) \equiv \exists y F_\alpha(x,y)$.

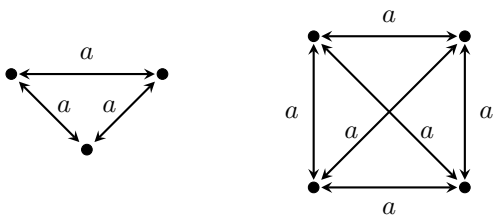
It is straightforward to show that the translation has the desired property.

Next we define a binary CRPQ $\varphi(x,y)$ that has no $\mathsf{GXPath}_{\text{reg}}$ equivalent.

$$\begin{aligned}\varphi(x,y) := (x,a,y) \wedge (x,a,z) \wedge (x,a,w) \wedge \\ (y,a,x) \wedge (z,a,x) \wedge (w,a,x) \wedge \\ (y,a,z) \wedge (y,a,w) \wedge \\ (z,a,y) \wedge (w,a,y) \wedge \\ (z,a,w) \wedge (w,a,z).\end{aligned}$$

Note that φ is stating that our graph has a complete subgraph of size four.

Next we take two graphs G_1 and G_2 as in the following figure.



G_1 G_2

Note that G_1 is a complete graph of three vertices with all the edges labeled a and G_2 is the same, but with four vertices. It is straightforward to see that $\varphi(G_1) = \emptyset$, while $\varphi(G_2) \neq \emptyset$.

It is well known that no $\mathcal{L}^3_{\infty\omega}$ sentence F can distinguish the two models (see, e.g., [31]). This is due to the fact that that duplicator has a winning strategy in an infinite 3-pebble game on these graphs, simply by preserving equality of pebbled elements. That is for any F we have $G_1 \models F$ iff $G_2 \models F$. Note that our result follows, since the above CRPQ selects the entire graph on G_2 and the empty graph on G_1. This completes our proof.

Proof of Proposition 4.7

From the previous theorem we know that there is a CRPQ not expressible in $\mathsf{GXPath}_{\text{reg}}$.

On the other hand, for any $\mathsf{GXPath}^{\text{pos}}_{\text{core}}$ expression e we can construct an equivalent U2CRPQ. That is, for any path expression α we define a U2CRPQ, named $\psi_\alpha(x,y)$, in two free variables, x and y, such that for any graph database G we have $[\![\alpha]\!]^G = \psi_\alpha(G)$. Similarly for any node expression φ we define a U2CRPQ $\psi_\varphi(x)$. We do so by induction on the structure of $\mathsf{GXPath}^{\text{pos}}_{\text{core}}$ expressions.

Basis:

- For $\alpha = \varepsilon$ we have $\psi_\alpha(x,y) := (x,\varepsilon,y)$.
- For $\alpha = \_$ we have $\psi_\alpha(x,y) := \bigvee_{a\in\Sigma}(x,a,y)$.
- For $\alpha = a$ we have $\psi_\alpha(x,y) := (x,a,y)$.
- For $\alpha = a^-$ we have $\psi_\alpha(x,y) := (x,a^-,y)$.
- For $\alpha = a^*$ we have $\psi_\alpha(x,y) := (x,a^*,y)$.
- For $\alpha = a^{-*}$ we have $\psi_\alpha(x,y) := (x,a^{-*},y)$.

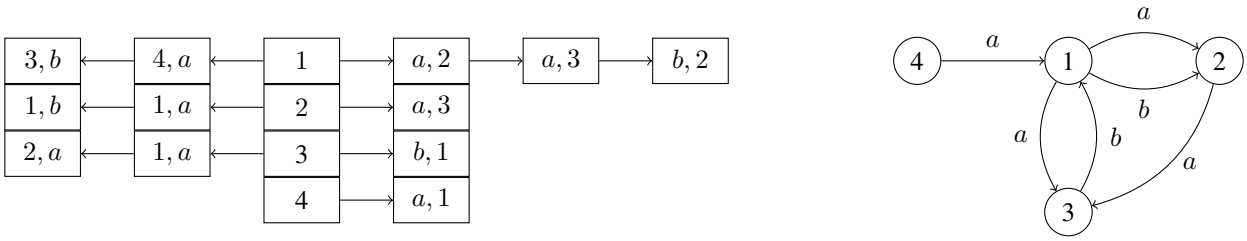


Figure 2: The adjacency list representation we assume for graphs for linear-time results in Section 5. The adjacency list is on the left and the corresponding graph on the right.

- For $\varphi = \top$ we have $\psi_\varphi(x) := \exists y(x, \varepsilon, y)$.

  Inductive step:
- For $\alpha = [\varphi]$ we have $\psi_\alpha(x, y) := (x, \varepsilon, y) \wedge \psi_\varphi(y)$.
- For $\alpha = \alpha' \cdot \beta'$ we have $\psi_\alpha(x, y) := \exists z \psi_{\alpha'}(x, z) \wedge \psi_{\beta'}(z, y)$.
- For $\alpha = \alpha' \cup \beta'$ we have $\psi_\alpha(x, y) := \psi_{\alpha'}(x, y) \vee \psi_{\beta'}(x, y)$.
- For $\varphi = \varphi_1 \wedge \varphi_2$ we have $\psi_\varphi(x) := \psi_{\varphi_1}(x) \wedge \psi_{\varphi_2}(x)$.
- For $\varphi = \varphi_1 \vee \varphi_2$ we have $\psi_\varphi(x) := \psi_{\varphi_1}(x) \vee \psi_{\varphi_2}(x)$.
- For $\varphi = \langle \alpha \rangle$ we have $\psi_\varphi(x) := \exists y \psi_\alpha(x, y)$.

It is straightforward to show that the defined expressions are equivalent.

Proof of Theorem 5.1

For obtaining the linear-time complexities in Theorem 5.1, we assume a total order "$\leq$" on the labels of edges. We assume that graphs are represented as adjacency lists in which we can perform the following operations in constant time:

- Given node v, get the adjacency list $(a_1, v_1), \ldots, (a_k, v_k)$ of outgoing edges, sorted in increasing order of labels. That is, $\{(a_1, v_1), \ldots, (a_k, v_k)\} = \{(a, v') \mid (v, a, v') \in E\}$ and, for each $i < j$ we have $a_i \leq a_j$.
- Given node v, get the adjacency list $(v_1, a_1), \ldots, (v_k, a_k)$ of incoming edges, sorted in increasing order of labels. That is, $\{(v_1, a_1), \ldots, (v_k, a_k)\} = \{(v', a) \mid (v', a, v) \in E\}$ and, for each $i < j$ we have $a_i \leq a_j$.

Figure 2 contains a graphical representation of an adjacency list representation of a graph that admits these operations. Furthermore, we assume a similar representation for NFAs. That is, if $\delta(q, a) = \{q_1, \ldots, q_n\}$ we assume that we can get the list $q_1, \ldots, q_n$ in constant time, given q and a.

We denote a *non-deterministic finite automaton* (NFA) over alphabet Σ as $A = (\Sigma, Q, \delta, I, F)$ where Q is a finite set of states, $\delta : Q \times \Sigma \to 2^Q$ is its transition function, $I \subseteq Q$ is the set of initial states, and $F \subseteq Q$ is the set of accepting states. By A^q we denote the NFA A in which the initial state set is replaced by $\{q\}$. The *language* $L(A)$ of an NFA A is defined as usual.

We start with a simple proposition that generalizes a construction in [38].

PROPOSITION 8.7. *Let $G = (V, E)$ be a directed, edge-labeled graph and $A = (\Sigma, Q, \delta, I, F)$ be an NFA. Furthermore, let $S \subseteq V$. Then we can compute the sets*

(a) $S_1 = \{v \in V \mid \exists$ path π from v to some $v' \in S$ such that $\lambda(\pi) \in L(A)\}$; and

(b) $S_2 = \{v \in V \mid \exists$ path π from some $v' \in S$ to v such that $\lambda(\pi) \in L(A)\}$,

in time $O(|V||Q| + |E||\delta|)$.

PROOF. All sets can be computed by interpreting G as an NFA and performing a product construction on G and A.

We first show (a). Intuitively, (a) is obtained by interpreting G as the NFA $N_G = (\Sigma, V, \delta_G, S, V)$ where δ_G maps every pair (v, a) onto $\{v' \mid (v, a, v') \in E\}$. The product construction can be done lazily without even constructing the entire product automaton. This can be done by dynamic programming as follows. We iteratively construct the set of pairs

$$P_1 = \{(v, q) \in V \times Q \mid \exists \text{ path } \pi \text{ from } v \text{ to some } v' \in S \text{ such that } \lambda(\pi) \in L(A^q)\}.$$

We initialize by taking $P_{1,0} = S \times F$ and, at each step, we compute

$$P_{1,i} = \{(v,q) \notin \cup_{j<i} P_{1,j} \mid \exists (v',q') \in P_{1,i-1} \text{ such that } (v,a,v') \in E \text{ and } q' \in \delta(q,a) \text{ for some } a \in \Sigma\}.$$

In order to compute $P_{1,i}$ efficiently, we can maintain a bit vector that remembers for each pair $(v,q) \in |V| \times |Q|$ if it is a member of $\cup_{j<i} P_{1,j}$. In addition, the adjacency list representation of graphs gives us in constant time, for each vertex $v' \in V$, the adjacency list $(v_1,a_1),\ldots,(v_k,a_k)$ of incoming edges to v' (i.e., all (v_j,a_j,v') are in E) in which the a_j are sorted. Similarly, in the NFA A we can obtain in constant time, for each state q', the list $(q_1,a'_1),\ldots,(q_\ell,a'_\ell)$ of incoming transitions to q' in which the a'_j are sorted. Therefore, we can perform a merge-join on the lists $((v_j,a_j))_{j=1}^{k}$ and $((q_j,a'_j))_{j=1}^{\ell}$ to compute $P_{1,i}$. If, for some i, $P_{1,i}$ is empty, then $P_1 = \cup_{j=0}^{i-1} P_{1,j}$ and we are done. Finally, the set S_1 is

$$\{v \in V \mid (v,q_0) \in P_1 \text{ for some } q_0 \in I\}.$$

The time complexity of the algorithm is $O(|V||Q|)$ for the storage of the bit vector, plus $O(e)$ for the computation of the set P_1, where e is proportional to the part of the product automaton of A and N_G from which a final state (i.e., a state in $S \times F$) can be reached. More formally, e is the cardinality of

$$\{\big((v_1,q_1),a,(v_2,q_2)\big) \mid \text{there is a path from } (v_1,q_1) \text{ to some } (v,q) \in S \times F, \text{ starting with } ((v_1,q_1),a,(v_2,q_2)) \text{ in } A \times N_G\}.$$

Notice that $e \leq |\delta||E|$ and can potentially be much smaller (and even much smaller than $|G|$). Furthermore, notice that we needed the edges to be sorted to achieve this complexity. If we do not assume this, then the complexity of the algorithm for computing P_1 would either be $O(|E||\delta||\Sigma|)$ (if we replace the merge-join by a naive nested loop join) or $O(|E|\log|E| + |\delta|\log|\delta| + e)$ (if we first sort everything and then perform this algorithm).

Part (b) is obtained by swapping out I and F, reversing all the transitions of the NFA A and applying (a). The time analysis is analogous as for (a). □

In the proof of Proposition 8.7, we only need $O(|V||Q|)$ for storing a $|V||Q|$-length bit vector that allows us to test if we visited a node before. Therefore, if we would store this data structure in a hash-table instead, we may be able to solve the two problems lazily and thereby consuming less than linear time in favorable cases. (In the spirit of local model checking.)

Proposition 8.7 is the core of a possible linear time algorithm for Theorem 5.1. We now extend NFAs and Proposition 8.7 to be able to take $\mathsf{GXPath}_{\text{reg}}^{\text{path-pos}}$ node expressions into account. Our extension of NFAs is similar to an idea in [38] and is tweaked to our needs. Let Σ^- be the set $\{a^- \mid a \in \Sigma\}$. We assume w.l.o.g. that Σ^- is disjoint from Σ. We denote $\Sigma^- \uplus \Sigma \uplus \{\_\}$ by $\hat{\Sigma}$. Moreover, let _ be a new symbol not occurring in Σ or Σ' which will denote the wildcard.

DEFINITION 8.8. *A* $\mathsf{GXPath}_{\text{reg}}^{\text{path-pos}}$-NFA *is an NFA* $A = (\hat{\Sigma} \uplus \Gamma \uplus \{\_\}, Q, \delta, I, F)$ *where* Γ *is a finite set of* $\mathsf{GXPath}_{reg}^{path\text{-}pos}$ *node tests.*

Let $G = (V,E)$ be an edge-labeled graph. The semantics of $\mathsf{GXPath}_{\text{reg}}^{\text{path-pos}}$-NFAs will be defined over *generalized paths in* G, i.e., paths that also include reverse edges. Formally, a generalized path from node v_1 to node v_n in G is a sequence

$$\pi = v_1 a_1 v_2 a_2 v_3 \ldots v_{n-1} a_{n-1} v_n$$

such that, for each $i < n$, if $a_i \in \Sigma$ then $(v_i,a_i,v_{i+1}) \in E$ and if $a_i = c^- \in \Sigma^-$ then $(v_{i+1},c,v_i) \in E$. We denote the set of generalized paths by $\hat{\Sigma}[V]^*$. We now define the *extended transition function* $\delta^* : Q \times \hat{\Sigma}[V]^* \to 2^Q$, inductively. For a state $q \in Q$ and path $\pi \in \hat{\Sigma}[V]^*$, we define $\delta^*(q,\pi)$ to be the smallest subset of Q such that all the following hold:

- if $\pi = v$, then $q \in \delta^*(q,v)$;
- if $\pi = v_1 a v_2$ with $a \in \hat{\Sigma}$, then $\delta(q,a) \subseteq \delta^*(q,v_1 a v_2)$ and $\delta(q,\_) \subseteq^* (q,v_1 a v_2)$;
- if $\pi = \pi' a v$ for some $\pi' \in \hat{\Sigma}[V]^*$, $a \in \hat{\Sigma}$, and if $q_1 \in \delta^*(q,\pi')$, then $\delta(q_1,a) \subseteq \delta^*(q,\pi)$ and $\delta(q_1,\_) \subseteq^* (q,\pi)$; and
- if π ends in node v and $q_1 \in \delta^*(q,\pi)$, then $\cup_{v \in [\![\varphi]\!]^G} \delta(q_1,\varphi) \subseteq \delta^*(q,\pi)$.

By $L(A)$ we denote the set of generalized paths π of G such that $\delta^*(q_0,\pi) \cap F \neq \emptyset$, for some $q_0 \in I$.

THEOREM 5.1: *Both* QUERY EVALUATION *and* QUERY COMPUTATION *problems for* $\mathsf{GXPath}_{reg}^{path\text{-}pos}$ *can be solved in linear time, i.e.,* $O(|\alpha| \cdot |G|)$.

PROOF SKETCH. Let $G = (V, E)$. The algorithm is recursive on the structure of path expressions. We first prove by induction on subexpressions of α that

- for each node subexpression φ, we can compute $[\![\varphi]\!]^G$ in time $O(|\varphi||G|)$ and,
- for each path subexpression β, we can compute $[\![\langle\beta\rangle]\!]^G$ in time $O(|\beta||G|)$.

Furthermore, we can store, for each $v \in V$, whether $v \in [\![\varphi]\!]^G$ (resp. $v \in [\![\langle\beta\rangle]\!]^G$) within the same time bound using a bit-vector B of length $|V||\alpha|$. As such, each node v and each subexpression φ has a corresponding bit in B, called the φ-bit of v in B.

The algorithm is a dynamic programming procedure that annotates nodes v of V with all subexpressions φ and β such that $v \in [\![\varphi]\!]^G$ or $v \in [\![\langle\beta\rangle]\!]^G$.

For proving the induction, we start with the observation that the base case for node expressions, i.e., $\varphi = \top$ is straightforward. For every node v, we set the φ-bit of v in B to 1.

In the induction step we consider path expressions and non-trivial node expressions.

- If $\varphi = \neg\psi$, then, for each $v \in V$, the φ-bit for v in V becomes the negation of the ψ-bit for v.
- If $\varphi = \psi_1 \wedge \psi_2$, then, for each $v \in V$, the φ-bit for v in V becomes the disjunction of the ψ_1- and ψ_2-bits for v.

If β is a $\mathsf{GXPath}_{\text{reg}}^{\text{path-pos}}$ expression, then we can convert β into an $\mathsf{GXPath}_{\text{reg}}^{\text{path-pos}}$-NFA A over alphabet $\{a, a^- \mid a \in \Sigma\} \cup \{[\varphi] \mid [\varphi]$ is an immediate subexpression of $\beta\}$. (Here, $[\varphi]$ is an *immediate* subexpression of β if it is not contained in another subexpression of the form ψ in β.) The construction of A is in linear time and follows the lines of the Thompson construction for converting regular expressions into equivalent NFAs. The size of A is linear in the size of β, minus the sum of the sizes of the immediate subexpressions $[\varphi]$. The automaton A has the property that $(v_1, v_2) \in [\![\beta]\!]^G$ if and only if there is a generalized path π from v_1 to v_2 in G with $\lambda(\pi) \in L(A)$. Similarly as Proposition 8.7, we can prove the following:

PROPOSITION 8.9. *Let $G = (V, E)$ be a directed, edge-labeled graph and A be a $\mathsf{GXPath}_{reg}^{path\text{-}pos}$-NFA. Assume that, for every Γ-symbol φ of A and node $v \in V$, we can determine in constant time whether $v \in [\![\varphi]\!]^G$. Furthermore, let $S \subseteq V$. Then we can compute the sets*

(a) $S_1 = \{v \in V \mid \exists$ *path π from v to some $v' \in S$ such that $\pi \in L(A)\}$; and*

(b) $S_2 = \{v \in V \mid \exists$ *path π from some $v' \in S$ to v such that $\pi \in L(A)\}$,*

in time $O(|V||Q| + |E||\delta|)$.

The proof of Proposition 8.9 is analogous to the proof of Proposition 8.7 but takes the extra symbols from Σ^- and Γ into account, which can be treated similarly as Σ-symbols.

When we take $S = V$ in Proposition 8.9, then we can compute the set S_1 in linear time. We set the β-bit for v to 1 if $v \in S_1$ and we set it to 0 otherwise.

Notice that, since the size of A is linear in the size of β minus the sum of the sizes of the immediate subexpressions $[\varphi]$, we can compute $[\![\langle\beta\rangle]\!]^G$ in time $O(|\beta||G|)$ overall.

Finally, if the input for QUERY COMPUTATION, is α and the set $S \subseteq V$, then we convert α to an automaton, similarly as before, apply Proposition 8.9, and return the set S_2. □

Proof of Theorem 5.4

THEOREM 5.4: *Both* QUERY EVALUATION *and* QUERY COMPUTATION *problems for $\mathsf{GXPath}_{reg}^{path\text{-}pos}(c)$ can be solved in linear time, i.e., $O(|\alpha| \cdot |G|)$.*

PROOF. We can do almost the exact same algorithm as the one above for Theorem 5.1. Indeed, if we meet a subexpression of the type $= c$ or $\neq c$, then we can easily compute $[\![= c]\!]^G$ and $[\![\neq c]\!]^G$ in linear time by performing a depth-first traversal through G. □

Proof of Theorem 5.3

We first show that we can do $\mathsf{GXPath}_{\text{reg}}$ in time $O(|\alpha| \cdot |G|^2)$.

THEOREM 8.10. *Both* QUERY EVALUATION *and* QUERY COMPUTATION *problems for* GXPath_{reg} *can be solved in polynomial time, specifically, i.e.,* $O(|\alpha| \cdot |G|^2)$.

PROOF. Notice that the only feature of GXPath_{reg} queries that is not present in the queries in Theorem 5.1 is path complementation, i.e., subqueries of the form $\overline{\beta}$ where β is a path query.

We prove by induction on the number of path complement operators in α that we can compute $[\![\alpha]\!]^G$ in time $O(|\alpha| \cdot |G|^2)$. Furthermore, the binary relation $[\![\alpha]\!]^G$ is sorted. (The primary sort key being its left column and the secondary sort key being its right column.)

When α does not contain any path complement operator, then the theorem follows quickly from Theorem 5.1. Indeed, we can compute the table representation of $[\![\alpha]\!]^G$ in time $O(|\alpha| \cdot |G|^2)$ by linearly many calls to Proposition 8.9(b). We iterate through all the nodes $v \in V$ (in order) and append the list $(v, v_1), \ldots, (v, v_k)$ to the output, where $S_2 = \{v_1, \ldots, v_k\}$. In the algorithm for Proposition 8.9 (and Proposition 8.7) we can maintain an additional bit vector of size $|V|$ in which we set a bit for some node v to 1 if we visit v in some state $q \in I$. The list S_2 is then obtained by outputting the true bits in the latter vector in order. The total complexity is $O(|V||\alpha||G|)$.

For the inductive case, we can assume that we have an expression of the form $\overline{\beta}$. By induction, we can assume that we already know a sorted binary relation for $[\![\beta]\!]^G$. Therefore, the result is obtained by traversing $[\![\beta]\!]^G$ in increasing order of node pairs, and writing a pair (v_1, v_2) to the table for $[\![\overline{\beta}]\!]^G$ if and only if does not occur in $[\![\beta]\!]^G$. Notice that we can output the nodes of $[\![\overline{\beta}]\!]^G$ in increasing order. Therefore, the total algorithm has complexity $O(|V||\alpha||G|)$. □

Now we prove Theorem 5.3:

THEOREM 5.3: *Both* QUERY EVALUATION *and* QUERY COMPUTATION *problems for* $\mathsf{GXPath}_{reg}(\mathsf{c}, \mathsf{eq})$ *can be solved in polynomial time, specifically, i.e.,* $O(|\alpha| \cdot |G|^2)$.

PROOF. As we said in the proof of Theorem 5.4, constant tests do not introduce extra complexity. Therefore we have a complexity of $O(|\alpha||G|)$ for $\mathsf{GXPath}_{reg}^{\text{path-pos}}$ with constant tests and $O(|\alpha||G|^2)$ for GXPath_{reg} with constant tests.

Now assume that we have equality tests of the form $\langle \beta_1 = \beta_2 \rangle$ and $\langle \beta_1 \neq \beta_2 \rangle$. In this case we perform the same algorithm as in Theorem 8.10 but we store some corresponding data values as well. In particular, for each path subexpression β we compute an additional table $[\![\beta]\!]^G_{\text{data}}$ containing all records $(v_1, v_2, \rho(v_2))$ sorted on the values of v_1 then on $\rho(v_2)$, and then on v_2. (We can, e.g., assume the order on data values to be the natural ordering on their representations as bit-strings.)

If we then need to compute the result for $\langle \beta_1 = \beta_2 \rangle$, we can do a merge-join on $[\![\beta_1]\!]^G_{\text{data}}$ and $[\![\beta_2]\!]^G_{\text{data}}$ on the first column and then (when the first column values are equal) on the third column. For every match, i.e., every pair of records $(v_1, v_2, \rho(v_2))$ from $[\![\beta_1]\!]^G_{\text{data}}$ and $(v_1, v_3, \rho(v_3))$ from $[\![\beta_2]\!]^G_{\text{data}}$ with $\rho(v_2) = \rho(v_3)$, we write v_1 into $[\![\langle \beta_1 = \beta_2 \rangle]\!]^G$. The result for $\langle \beta_1 \neq \beta_2 \rangle$ can be computed similarly.

We now prove that we can compute the tables $[\![\beta]\!]^G_{\text{data}}$ in time $O(|\alpha||G|^2)$. To this end, we start our algorithm with a one-time computation where we sort all nodes in G according to their data values. This takes time $O(|V| \log |V|)$ and allows us to construct a vector o of integers of length $|V|$ in which for every node v, we have $o(v) = k$ if the data value of v is the k-th value in the sorted order. That is, given a node v, we can obtain the number k in constant time. With the vector o, we can update the procedure in the proof of Theorem 8.10 to compute $[\![\beta]\!]^G_{\text{data}}$. Now, we need to be able to obtain the vector S_2 in increasing order of data values. We do this by maintaining a new vector of size $|V|$ and whenever we would insert v into S_2, we write v at position $o(v)$ in this vector. The ordered set S_2 is then represented by this bit vector at the end of the algorithm. Altogether, this allows us to compute $[\![\beta]\!]^G_{\text{data}}$ in time $O(|\beta||G|^2)$. □

Proof of Theorem 5.2

PROOF OF THEOREM 5.2: *Both* QUERY EVALUATION *and* QUERY COMPUTATION *problems for* $\#\mathsf{GXPath}_{reg}(\mathsf{c}, \mathsf{eq})$ *can be solved in polynomial time, specifically, i.e.,* $O(|\alpha| \cdot |G|^3)$.

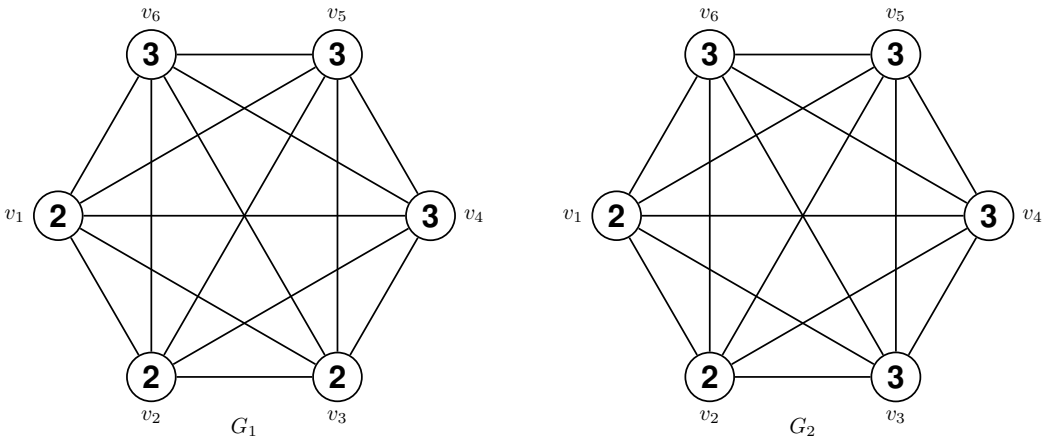
PROOF. We do everything the same as in the proof of Theorem 5.4, but we additionally need to handle counters. To this end, we explain how we can compute a table for $[\![\beta^{n,m}]\!]^G_{\text{data}}$, given the table for $[\![\beta]\!]^G_{\text{data}}$. This can in fact be done similarly as in [33]: One can consider the connectivity matrix of the table and compute the new table by fast squaring on matrices. Getting sorted relations out of the connectivity matrices is trivial. (Alternatively, one could also compute the new table by implementing fast squaring directly on the tables, i.e., by performing $\log m$ join operations on the tables.) □

Proof of Proposition 6.1

We will first prove the result without constant tests.

To prove that $a_=$ is not expressible in $\mathsf{GXPath}_{\text{reg}}(\mathsf{eq})$ over graphs we will give two graphs G_1 and G_2, such that $[\![a_=]\!]^{G_1} \neq [\![a_=]\!]^{G_2}$, but for every $\mathsf{GXPath}_{\text{reg}}(\mathsf{eq})$ query e we have $[\![e]\!]^{G_1} = [\![e]\!]^{G_2}$.

Both G_1 and G_2 will be the graphs K_6, that is the complete graphs with six vertices and with data values $2, 2, 2, 3, 3, 3$ and $2, 2, 3, 3, 3, 3$, respectively, attached to the nodes. The graphs G_1 and G_2 are pictured in the following image.



It follows from the definitions that $(v_2, v_3) \in [\![a_=]\!]^{G_1}$, while $(v_2, v_3) \notin [\![a_=]\!]^{G_2}$. We conclude that $[\![a_=]\!]^{G_1} \neq [\![a_=]\!]^{G_2}$.

We now show that for any $\mathsf{GXPath}_{\text{reg}}(\mathsf{eq})$ query e we have $[\![e]\!]^{G_1} = [\![e]\!]^{G_2}$. In particular we show the following:

- For any path query α one of the following holds:
  - $[\![\alpha]\!]^{G_1} = [\![\alpha]\!]^{G_2} = \emptyset$, or
  - $[\![\alpha]\!]^{G_1} = [\![\alpha]\!]^{G_2} = Id(G_1)$, or
  - $[\![\alpha]\!]^{G_1} = [\![\alpha]\!]^{G_2} = {G_1}^2$, or
  - $[\![\alpha]\!]^{G_1} = [\![\alpha]\!]^{G_2} = {G_1}^2 - Id(G_1)$.
- For any node query φ one of the following holds:
  - $[\![\varphi]\!]^{G_1} = [\![\varphi]\!]^{G_2} = \emptyset$, or
  - $[\![\varphi]\!]^{G_1} = [\![\varphi]\!]^{G_2} = G_1$.

As before $Id(G_1)$ stands for the set $\{(x, x) : x \in G_1\}$. Note that since the sets of nodes of G_1 and G_2 are the same (and the graphs are not isomorphic because of the different data values), we can write $[\![\varphi]\!]^{G_2} = G_1$ and other claims.

We prove this claim by induction on the structure of our $\mathsf{GXPath}_{\text{reg}}(\mathsf{eq})$ expression e.

The base cases trivially follow. For the induction step assume that our claim is true for the expressions of lower complexity. We proceed by cases.

- If $\alpha = [\varphi]$ then by the inductive hypothesis we have two cases.
  - Either $[\![\varphi]\!]^{G_1} = [\![\varphi]\!]^{G_2} = \emptyset$, in which case $[\![\alpha]\!]^{G_1} = [\![\alpha]\!]^{G_2} = \emptyset$,
  - Or $[\![\varphi]\!]^{G_1} = [\![\varphi]\!]^{G_2} = G_1$, in which case $[\![\alpha]\!]^{G_1} = [\![\alpha]\!]^{G_2} = Id(G_1)$.
- If $\alpha = \alpha' \cup \beta'$ then the claim follows from the induction hypothesis and the fact that the set $\{\emptyset, {G_1}^2, {G_1}^2 - Id(G_1), Id(G_1)\}$ is closed under taking unions.
- If $\alpha = \alpha' \cdot \beta'$ we proceed as follows.
  Note first that $[\![\alpha]\!]^{G_1} = \emptyset$ iff $[\![\alpha']\!]^{G_1} = \emptyset$ or $[\![\beta']\!]^{G_1} = \emptyset$ (this follows from the inductive hypothesis about the structure of the answers, since for any other case the sets have nonempty composition). This is now equivalent to the same being true in G_2 and thus to $[\![\alpha]\!]^{G_2} = \emptyset$.
  If $[\![\alpha]\!]^{G_1} \neq \emptyset$ then we know that both $[\![\alpha']\!]^{G_1}$ and $[\![\beta']\!]^{G_1}$ belong to $\{{G_1}^2, {G_1}^2 - Id(G_1), Id(G_1)\}$. The claim now simply follows from the inductive hypothesis and the fact that the set $\{{G_1}^2, {G_1}^2 - Id(G_1), Id(G_1)\}$ is closed under composition of relations.

- If $\alpha = \overline{\alpha'}$ we have four cases.
  - In case that $[\![\alpha']\!]^{G_1} = [\![\alpha']\!]^{G_2} = \emptyset$ we have $[\![\alpha]\!]^{G_1} = [\![\alpha]\!]^{G_2} = {G_1}^2$.
  - In case that $[\![\alpha']\!]^{G_1} = [\![\alpha']\!]^{G_2} = {G_1}^2$ we have $[\![\alpha]\!]^{G_1} = [\![\alpha]\!]^{G_2} = \emptyset$.
  - In case that $[\![\alpha']\!]^{G_1} = [\![\alpha']\!]^{G_2} = {G_1}^2 - Id(G_1)$ we have $[\![\alpha]\!]^{G_1} = [\![\alpha]\!]^{G_2} = Id(G_1)$.
  - In case that $[\![\alpha']\!]^{G_1} = [\![\alpha']\!]^{G_2} = Id(G_1)$ we have $[\![\alpha]\!]^{G_1} = [\![\alpha]\!]^{G_2} = {G_1}^2 - Id(G_1)$.
- If $\alpha = {\alpha'}^*$ we have the same situation as in the previous case. In particular we know that transitive closures in each case will be the same.
- If $\varphi = \neg\varphi$ we have the following.
  - In case that $[\![\varphi']\!]^{G_1} = [\![\varphi']\!]^{G_2} = G_1$ we have $[\![\varphi]\!]^{G_1} = [\![\varphi]\!]^{G_2} = \emptyset$.
  - In case that $[\![\varphi']\!]^{G_1} = [\![\varphi']\!]^{G_2} = \emptyset$ we have $[\![\varphi]\!]^{G_1} = [\![\varphi]\!]^{G_2} = G_1$.
- If $\varphi = \varphi' \wedge \psi'$ the claim easily follows.
- If $\varphi = \langle\alpha\rangle$ we consider the value of $[\![\alpha]\!]^{G_1}$.
  - In case that $[\![\alpha]\!]^{G_1} = [\![\alpha]\!]^{G_2} = \emptyset$ we get $[\![\varphi]\!]^{G_1} = [\![\varphi]\!]^{G_2} = \emptyset$.
  - In case that $[\![\alpha]\!]^{G_1} = [\![\alpha]\!]^{G_2} = {G_1}^2, Id(G_1)$, or ${G_1}^2 - Id(G_1)$ we get $[\![\varphi]\!]^{G_1} = [\![\varphi]\!]^{G_2} = G_1$.
- If $\varphi = \langle\alpha = \beta\rangle$ we proceed by cases, depending of the value of $[\![\alpha]\!]^{G_1}$ and $[\![\beta]\!]^{G_1}$.
  Note that if either equals $\emptyset$ we get that $[\![\varphi]\!]^{G_1} = [\![\varphi]\!]^{G_2} = \emptyset$. There are now nine possible cases remaining.
  1. $[\![\alpha]\!]^{G_1} = [\![\alpha]\!]^{G_2} = Id(G_1)$ and $[\![\beta]\!]^{G_1} = [\![\beta]\!]^{G_2} = Id(G_1)$ implies that $[\![\varphi]\!]^{G_1} = [\![\varphi]\!]^{G_2} = G_1$.
  2. $[\![\alpha]\!]^{G_1} = [\![\alpha]\!]^{G_2} = Id(G_1)$ and $[\![\beta]\!]^{G_1} = [\![\beta]\!]^{G_2} = {G_1}^2$ implies that $[\![\varphi]\!]^{G_1} = [\![\varphi]\!]^{G_2} = G_1$.
  3. $[\![\alpha]\!]^{G_1} = [\![\alpha]\!]^{G_2} = Id(G_1)$ and $[\![\beta]\!]^{G_1} = [\![\beta]\!]^{G_2} = {G_1}^2 - Id(G_1)$ implies that $[\![\varphi]\!]^{G_1} = [\![\varphi]\!]^{G_2} = G_1$.
  4. All the remaining cases have the same result.
- If $\varphi = \langle\alpha \neq \beta\rangle$ we proceed by cases, depending of the value of $[\![\alpha]\!]^{G_1}$ and $[\![\beta]\!]^{G_1}$.
  Note that if either equals $\emptyset$ we get that $[\![\varphi]\!]^{G_1} = [\![\varphi]\!]^{G_2} = \emptyset$. Just as for $\langle\alpha = \beta\rangle$ we have nine cases. It is easily verified that we have $[\![\varphi]\!]^{G_1} = [\![\varphi]\!]^{G_2} = G_1$ for each case, except when $[\![\alpha]\!]^{G_1} = [\![\alpha]\!]^{G_2} = Id(G_1)$ and $[\![\beta]\!]^{G_1} = [\![\beta]\!]^{G_2} = Id(G_1)$. In this case we get $[\![\varphi]\!]^{G_1} = [\![\varphi]\!]^{G_2} = \emptyset$.

To extend the induction to work for constants, we assume the contrary. Let the e be an expression defining $a_=$. We exchange the data values 2 and 3 in our graphs G_1 and G_2 by any two data values that do not appear as constants in e. The proof is now the same as in the case without constants.

This completes the proof.

Proof of Theorem 6.3

PROOF OF THEOREM 6.3: *Both* QUERY EVALUATION *and* QUERY COMPUTATION *problems for* $\mathsf{GXPath}_{reg}(\mathsf{c}, \mathsf{eq}, \sim)$ *can be solved in polynomial time, specifically, i.e.,* $O(|\alpha| \cdot |G|^2)$.

PROOF. To see this we take the algorithm for $\mathsf{GXPath}_{\text{reg}}(\mathsf{eq})$ from Theorem 5.3 and modify it so that any time when we meet a subexpression of the form $\beta_=$, we walk through the table for $[\![\beta]\!]^G$ and remove all tuples with different data values, thus obtaining a table for $[\![\beta_=]\!]^G$. Similarly for $[\![\beta_{\neq}]\!]^G$. Notice that these operations do not influence the ordering of tuples in tables. □