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Main Track

Containment of Simple Conjunctive Regular Path Queries

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Abstract

Testing containment of queries is a fundamental reasoning task in knowledge representation. We study here the containment problem for Conjunctive Regular Path Queries (CRPQs), a navigational query language extensively used in ontology and graph database querying. While it is known that containment of CRPQs is EXPSPACE-complete in general, we focus here on severely restricted fragments, which are known to be highly relevant in practice according to several recent studies. We obtain a detailed overview of the complexity of the containment problem, depending on the features used in the regular expressions of the queries, with completeness results for NP, Π_2^p, PSPACE or EXPSPACE.

1 Introduction

Querying knowledge bases is one of the most important and fundamental tasks in knowledge representation. Although much of the work on querying knowledge bases is focused on conjunctive queries, there is often the need to use a simple form of recursion, such as the one provided by regular path queries (RPQ), which ask for paths defined by a given regular language. Conjunctive RPQs (CRPQs) can then be understood as the generalization of conjunctive queries with this form of recursion. CRPQs are part of SPARQL, the W3C standard for querying RDF data, including well known knowledge bases such as DBpedia and Wikidata. In particular, RPQs are quite popular for querying Wikidata. They are used in over 24% of the queries (and over 38% of the unique queries), according to recent studies (Malyshev et al. 2018; Bonifati, Martens, and Timm 2019). More generally, CRPQs are basic building blocks for querying graph-structured databases (Barceló 2013).

As knowledge bases become larger, reasoning about queries (e.g. for optimization) becomes increasingly important. One of the most basic reasoning tasks is that of query containment: is every result of query Q_1 also returned by Q_2? This can be a means for query optimization, as it may allow to avoid evaluating parts of a query, or reduce and simplify the query with an equivalent one. Furthermore, query containment has proven useful in knowledge base verification, information integration, integrity checking, and cooperative answering (Calvanese et al. 2000).

The containment problem for CRPQs is EXPSPACE-complete, as was shown by (Calvanese et al. 2000) in a now 'classical' KR paper, which appeared 20 years ago. However, the lower bound construction of Calvanese et al. makes use of CRPQs which have a simple shape (if seen as a graph of atoms) but contain rather involved regular expressions, which do not correspond to RPQs how they typically occur in practice. Indeed, the analyses of (Bonifati, Martens, and Timm 2019; Bonifati, Martens, and Timm 2020) reveal that a large majority of regular expressions of queries used in practice are of a very simple form. This motivates us to revisit CRPQ containment on queries, focusing on commonly used kinds of regular expressions. Our goal is to identify restricted fragments of CRPQs that are common in practice and which have a reasonable complexity for query containment.

Contribution. According to recent studies on query logs, investigating over 500 million SPARQL queries (Bonifati, Martens, and Timm 2019; Bonifati, Martens, and Timm 2020), it turns out that a large majority of regular expressions that are used for graph navigation are of rather simple forms, like a^*, ab^*, $(a+b)c^*$, $a(b+c)^*d$, i.e., concatenations of (disjunctions of) single symbols and Kleene stars of (disjunctions of) single symbols. Since CRPQs have concatenations built-in, CRPQs with such expressions are essentially CRPQs in which every atom has a regular expression of the form $(a_1 + \cdots + a_n)$ or $(a_1 + \cdots + a_n)^*$ for $n \geq 1$. In the remainder of the paper, we often abbreviate the former type of atom with A and the latter by A^*. If $n = 1$, we write a and a^*. Table 1 gives an overview of the frequency of such expressions in the following data sets:

(a) The data set studied by (Bielefeldt, Gonsior, and Krötzsch 2018; Bonifati, Martens, and Timm 2019), which was released by (Malyshev et al. 2018) and contains 208 million parseable Wikidata queries, with over 55 million regular path queries.
(b) The data set of (Bonifati, Martens, and Timm 2020), which contains 339 million parseable queries, mostly from DBpedia, but also from LinkedGeoData, BioPortal, OpenBioMed, Semantic Web Dog Food and the British Museum. These queries contain around 1.5 million regular path queries.[1]

[1]One sees that regular path queries are much more common in the Wikidata log than in the (mainly) DBpedia log. The reason for this is that the graph structure of DBpedia was designed before

When we list multiple types of atoms in the table, we allow concatenations of these types. So, $a(b+c)^*d$ is of type a, A^* and also of the more general type A, A^*. In contrast to the types listed, RPQs that are merely concatenations of single symbols, e.g., abc or aa, represent only about 25% of the valid Wikidata expressions and 7% of the valid DBpedia$^\pm$ expressions in the table.

Another motivation to study CRPQs with atoms of the forms a, a^*, A, and A^* is that these are currently the only expressible atoms in CRPQs in Cypher 9 (Francis et al. 2018, Figure 3), a popular query language for property graphs.

We study the complexity of CRPQ containment for such fragments $\mathcal{F}$ of "simple CRPQs", that is, CRPQs that only use atoms of some of the types a, a^*, A, and A^*. For each fragment $\mathcal{F}$, we provide a complete picture of the complexities of containment problems of the form $\mathcal{F} \subseteq \mathcal{F}$, $\mathcal{F} \subseteq$ CRPQ, and CRPQ $\subseteq \mathcal{F}$ (cf. Table 2, which we discuss in Section 3 in detail). The main take-aways are:

1. Even for such simple CRPQs, containment of the form $\mathcal{F} \subseteq \mathcal{F}$ can become EXPSPACE-complete. Moreover, this lower bound already holds for containment of CRPQs using only a-atoms and A^*-atoms. This was surprising to us, because such CRPQs seem at first sight to be only mild extensions of conjunctive queries: they extend conjunctive queries only with atoms of the form $(a_1 + \cdots + a_n)^*$, i.e., Kleene closures over sets of symbols. The contrast between NP-completeness of containment for conjunctive queries and EXPSPACE-completeness for CRPQs that additionally allow $(a_1 + \cdots + a_n)^*$ is quite striking.
2. As soon as we disallow disjunction within Kleene closures in $\mathcal{F}$, the complexity of the abovementioned containment problems drops drastically to Π_2^p or PSPACE. The good news is that such regular expressions are still extremely common in practice, e.g., over 98% of the RPQs in the Wikidata query logs (Table 1).

Due to the page limit, we can only provide sketches of some of the proofs. A version with more extensive proofs is available at https://arxiv.org/abs/2003.04411 (Figueira et al. 2020).

Organization In Section 2 we introduce the necessary notation. In Section 3 we present our main results which are then proved in Sections 4–7. We discuss related work in detail in Section 8 and we conclude in Section 9.

2 Preliminaries

Let Σ be an infinite set of **labels**, to which we sometimes also refer as the **alphabet**. We abstract knowledge bases (or KBs, knowledge graphs, or graph databases) as finite, edge-labeled directed graphs $K = (V, E)$, where V is a finite nonempty set of nodes, and E is a set of labeled directed edges $(u, a, v) \in V \times \Sigma \times V$. A **path** is a (possibly empty) sequence $\pi = (v_0, a_1, v_1) \cdots (v_{n-1}, a_n, v_n)$ of edges; we say that π is a path from v_0 to v_n. The **length** of π is the number $n \geq 0$ of edges in the sequence. We denote by $lab(\pi)$ the word $a_1 \cdots a_n$ of edge labels seen along the path.

RPQs (property paths) existed in SPARQL.

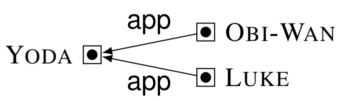
If all edges of π have the same label $a \in \Sigma$, we say π is an **a-path**. By ε we denote the empty word. Regular expressions are defined as usual. We use uppercase letters R for regular expressions and denote their language by $L(R)$.

A **conjunctive regular path query** (**CRPQ**) has the general form $Q(x_1, \ldots, x_n) \leftarrow A_1 \wedge \ldots \wedge A_m$. The **atoms** $A_1, \ldots, A_m$ are of the form yRz, where y and z are variables and R is a regular expression. Each **distinguished variable** x_j from the left hand side has to occur in some atom on the right hand side. A **homomorphism** from Q to K is a mapping μ from the variables of Q to V. Such a homomorphism **satisfies** an atom xRy if there is a path from $\mu(x)$ to $\mu(y)$ in K which is labeled with a word in $L(R)$. A homomorphism from Q to K is called a **satisfying homomorphism** if it satisfies each atom A_i. For brevity, we also use the term **embedding** for satisfying homomorphisms. The set of **answers** $ans(Q, K)$ of a CRPQ Q over a knowledge base K is the set of tuples $(d_1, \ldots, d_n)$ of nodes of K such that there exists a satisfying homomorphism for Q on K that maps x_i to d_i for every $1 \leq i \leq n$.

Given two CRPQs Q_1, Q_2, we say that Q_1 is **contained** in Q_2, denoted by $Q_1 \subseteq Q_2$, if $ans(Q_1, K) \subseteq ans(Q_2, K)$ for every knowledge base K. We say Q_1 is **equivalent** to Q_2, denoted by $Q_1 \equiv Q_2$, if $Q_1 \subseteq Q_2$ and $Q_2 \subseteq Q_1$. We study the following problem, for various fragments $\mathcal{F}_1, \mathcal{F}_2$ of CRPQ.

Containment of $\mathcal{F}_1$ in $\mathcal{F}_2$	
Given:	Two queries $Q_1 \in \mathcal{F}_1$, $Q_2 \in \mathcal{F}_2$.
Question:	Is $Q_1 \subseteq Q_2$?

Example. To illustrate query containment we consider the following example. Let $Q_1(x_1, x_2) \leftarrow (x_1\ \mathsf{app}\ jm_1) \wedge (x_2\ \mathsf{app}\ jm_1) \wedge (jm_1\ \mathsf{app}\ jm_2)$. Query Q_1 returns (x_1, x_2) only if they were both the apprentices of jm_1 (a Jedi master) who was in turn an apprentice of jm_2. Now consider $Q_2(x_1, x_2) \leftarrow (x_1\ \mathsf{app}{\cdot}\mathsf{app}\ jm) \wedge (x_2\ \mathsf{app}{\cdot}\mathsf{app}\ jm)$. We see that $Q_1 \subseteq Q_2$. However if we remove the last atom from Q_1, $Q_1 \subseteq Q_2$ is not necessarily true. The following database provides a counterexample. Q_1 without the last



atom returns (LUKE, OBI-WAN) though Q_2 does not. ■

Let Q be the CRPQ $Q(x_1, \ldots, x_n) \leftarrow y_1 R_1 y_2 \wedge \ldots \wedge y_{2m-1} R_m y_{2m}$. Let K be a knowledge base and ν a total mapping from the variables $\{x_1, \ldots, x_n, y_1, \ldots, y_{2m}\}$ of Q to the nodes of K. Then K is **ν-canonical** for Q if

- K consists of m simple paths, one for each atom of Q, which are node- and edge-disjoint except for the start and end nodes, and
- for each $i \in \{1, \ldots, m\}$ the simple path π_i associated to the atom $y_{2i-1} R_i y_{2i}$ connects the node $\nu(y_{2i-1})$ to the node $\nu(y_{2i})$ and has $lab(\pi_i) \in L(R_i)$.

It is easy to see that $Q_1 \not\subseteq Q_2$ iff there exists a knowledge base K and a mapping ν from the variables of Q_1 to the

	Wikidata Queries				DBpedia$^{\pm}$ Queries			
	One-way RPQs		Two-way RPQs		One-way RPQs		Two-way RPQs	
RPQ Class	Valid %	Unique %	Valid %	Unique %	Valid %	Unique %	Valid %	Unique %
A, A^*	99.02%	98.73%	99.83%	99.83%	68.99%	47.41%	94.35%	82.86%
A, a^*	98.40%	98.31%	99.22%	99.44%	65.29%	46.02%	75.00%	76.44%
a, A^*	93.50%	95.99%	94.30%	97.10%	64.27%	31.37%	89.51%	66.53%
a, a^*	92.88%	95.58%	93.69%	96.69%	60.57%	29.97%	65.87%	44.45%
Total	55,333K	14,189K	55,333K	14,189K	1,529K	405K	1,529K	405K

Table 1: Percentage of simple RPQs and 2RPQs in the Wikidata query logs in the study (Bonifati, Martens, and Timm 2019) (left) and the diverse query logs of (Bonifati, Martens, and Timm 2020) (right). For every analysis, we show percentages on all valid queries (Valid) and on all valid queries after duplicate elimination (Unique).

$\mathcal{F}$	$\mathcal{F} \subseteq \mathcal{F}$	$\mathcal{F} \subseteq$ CRPQ	CRPQ $\subseteq \mathcal{F}$
a	NP (†)	NP (4.2)	Π_2^p (4.4)
A	Π_2^p (4.3)	Π_2^p	PSPACE (4.5)
(a, a^*)	Π_2^p (‡)	Π_2^p	PSPACE (5.3)
(A, a^*)	Π_2^p	Π_2^p (5.2)	PSPACE (5.5)
(a, A^*)	EXPSPACE (6.1)	EXPSPACE	EXPSPACE
(A, A^*)	EXPSPACE	EXPSPACE ($\star$)	EXPSPACE ($\star$)

Table 2: Complexity of Containment of different fragments $\mathcal{F}$ of CRPQs. All results are complete for the class given. We provide references in round brackets. When there is no bracket, the result follows directly from another cell in the table. (†): (Chandra and Merlin 1977), (‡): (Deutsch and Tannen 2002, fragment (l^*)), ($\star$): (Calvanese et al. 2000)

nodes of K such that (i) K is ν-canonical for Q_1 and (ii) $(\nu(x_1), \ldots, \nu(x_n)) \notin ans(Q_2, K)$. Therefore, to decide Containment, it suffices to study containment on knowledge bases which are ν-canonical for Q_1. We call these knowledge bases **canonical models** of Q_1.

It is well-known that there is a natural correspondence between (the bodies of) CRPQs and graphs by viewing their variables as nodes and the atoms as edges. We will therefore sometimes use terminology from graphs for CRPQs (e.g., connected components).

3 Main Results

For a class of regular languages $\mathcal{L}$ we write CRPQ($\mathcal{L}$) to denote the set of CRPQs whose languages (of regular expressions in atoms) are in $\mathcal{L}$. We use the same abbreviations for $\mathcal{L}$ as discussed in the Introduction: a for regular expressions that are just a single symbol, a^* for Kleene closures of a single symbols, A for disjunctions (or sets) of symbols, and A^* for Kleene closures of disjunctions (or sets) of symbols. A sequence of abbreviations in $\mathcal{L}$ represents options: for instance, CRPQ(a, A^*) is the set of CRPQs in which each atom uses either a single symbol or a transitive closure of a disjunction of symbols.[2]

[2]In some proofs, we also allow concatenations of these forms. But this does not make a difference: in CRPQs such concatenations can always be eliminated at the cost of a few extra variables.

In this paper, we give a complete overview of the complexity of containment for the fragments $\mathcal{F}$ = CRPQ(a), CRPQ(A), CRPQ(a, a^*), CRPQ(A, a^*), CRPQ(a, A^*), and CRPQ(A, A^*). That is, for each of these fragments we prove that their containment problem is complete for NP, Π_2^p, or EXPSPACE. Furthermore, for each of these fragments $\mathcal{F}$, we give a complete overview of the complexity of the containment problems of the form $\mathcal{F} \subseteq$ CRPQ and CRPQ $\subseteq \mathcal{F}$. An overview of our results can be found in Table 2. All results are completeness results. Some of the results were already obtained in other papers, which we indicate in the table.

Interestingly, our results imply that containment is EXPSPACE-complete only if we allow sets of symbols under the Kleene star both in the left- and right-hand queries. As soon as we further restrict the usage of the Kleene star on one side, the complexity drops to PSPACE or even Π_2^p. As it turns out, queries having a^* as only means of recursion is still very representative of the queries performed in practice, as evidenced in Table 1, where over 98% of the RPQs in the Wikidata logs are of this form. In the DBpedia$^{\pm}$ logs, this percentage is still around 70% of the total RPQs. Two main reasons why this percentage is lower here are that "wildcards" of the form $!a$, i.e., follow an edge *not* labeled a, and 2RPQs of the form $(a + \hat{}a)^*$, i.e., undirected reachability over a-edges, make up around 15% and 20% respectively of the expressions in unique queries in DBpedia$^{\pm}$. The fact that equivalence testing is Π_2^p for these queries, gives hope that optimizations by means of static analysis may be practically feasible for most of the CRPQ used for querying ontologies and RDF data.

Our results apply to both finite and infinite sets of labels, if we do not explictly say otherwise. The reason is that as long as the query language does not allow for wildcards, we can always restrict to the symbols explicitly used in the queries, which is always a finite set.

If wildcards are allowed, the complexity of query containment can heavily depend on the finiteness of the alphabet of edge labels Σ. We discovered that our techniques can be used to settle an open question (and correct an error) in the work of Deutsch and Tannen (2002), who have also considered containment of simple CRPQs. Deutsch and Tannen considered CRPQ fragments motivated by the navigational features of XPath and claimed that containment for their *W-fragment* (see Section 7 for a definition), using infinite alphabets, is PSPACE-hard. However, we prove that containment for this fragment is in Π_2^p (Theorem 7.1). The minor error is that Deutsch and Tannen assumed *finite* alphabets in their hardness proof. In fact, when one indeed assumes a finite set of edge labels in KBs, we prove that the containment problem for the W-fragment is EXPSPACE-complete (Proposition 7.2).

4 No Transitive Closure

In this section we study simple CRPQ fragments without transitive closure. We first observe that CRPQ(a) is equivalent to the well-studied class of conjunctive queries (CQ) on binary relations.

Theorem 4.1 (Chandra and Merlin 1977)**.** *Containment of* CRPQ(a) *in* CRPQ(a) *is* NP*-complete.*

Even when we allow arbitrary queries on the right, the complexity stays the same. The reason is that the left query has a single canonical model K of linear size, and thus we can check containment by testing for a satisfying homomorphism from Q_2 to K (that preserves the distinguished nodes).

Theorem 4.2. *Containment of* CRPQ(a) *in* CRPQ *is* NP*-complete.*

If we allow more expressive queries on the left, the complexity becomes Π_2^p, even if the right-hand queries are CQs.

Theorem 4.3. *Containment of* CRPQ(A) *in* CRPQ(a) *is* Π_2^p*-complete, even if the size of the alphabet is fixed.*

Proof sketch. The upper bound is immediate from Corollary 5.2, which in turn follows from Theorem 7.1. Both these results are proved later. For the lower bound, we reduce from $\forall\exists$-QBF (i.e., Π_2-Quantified Boolean Formulas). Let

$$\Phi \;=\; \forall x_1,\ldots,x_n\;\exists y_1,\ldots,y_\ell\;\varphi(x_1,\ldots,x_n,y_1,\ldots,y_\ell)$$

be an instance of $\forall\exists$-QBF such that φ is quantifier-free and in 3-CNF. We construct boolean queries Q_1 and Q_2 such that $Q_1 \subseteq Q_2$ if, and only if, Φ is satisfiable.

The query Q_1 is defined in Figure 2, over the alphabet of labels $\{a, x_1, \ldots, x_n, y_1, \ldots, y_\ell, t, f\}$. We now explain how we define Q_2, over the same alphabet. Every clause of Φ is represented by a subquery in Q_2, as depicted in Figure 3. All nodes with identical label ($y_{1,t}$ and $y_{1,f}$ in gadgets D, E) in Figures 2 and 3 are the same node. (So, both queries are DAG-shaped.) Note that for every clause and every existentially quantified literal y_i therein we have one node named $y_{i,tf}$ in Q_2. The E-gadget is designed such that every represented literal can be homomorphically embedded, while exactly one literal has to be embedded in the D-gadget.

The intuitive idea is that the valuation of the x-variables is given by the concrete canonical model K (i.e., whether the corresponding edge is labeled t or f in the D gadget), while the valuation of the y-variables is given by the embedding of Q_2 into K (i.e., whether the corresponding node is embedded into the node $y_{\llcorner,t}$ or $y_{\llcorner,f}$). The embedding of y-variables across several clauses has to be consistent, as all

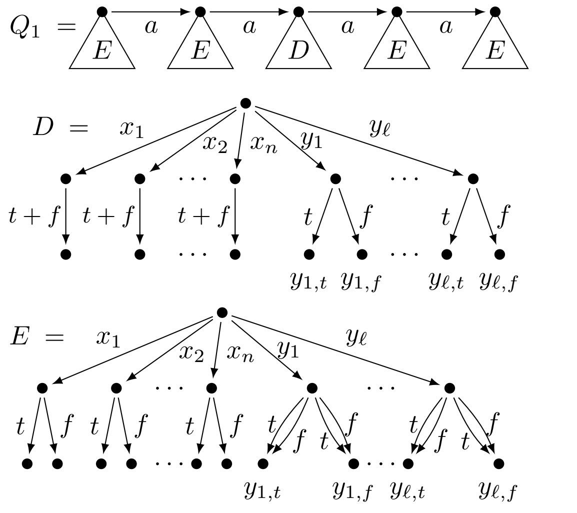


Figure 2: Query Q_1 used in the proof of Theorem 4.3 and the gadgets D and E used in Q_1.

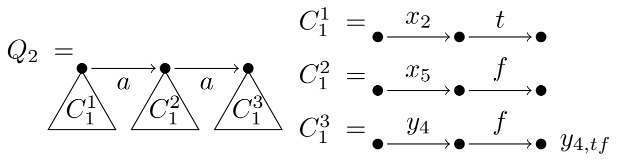


Figure 3: Example of Q_2 in the proof of Theorem 4.3 for the formula $\varphi = (x_2 \vee \neg x_5 \vee \neg y_4)$.

clauses share the same nodes $y_{\llcorner,tf}$, which uniquely get embedded either into $y_{\llcorner,t}$ or $y_{\llcorner,f}$. Hence, when the formula Φ is satisfiable, for any assignment to the variables $\{x_i\}$ (given by the choice of *t*/*f* edges in D), there is a mapping from $y_{\llcorner,tf}$ to one of $y_{\llcorner,f}$ or $y_{\llcorner,t}$. This gives $Q_1 \subseteq Q_2$. Conversely, if Q_2 can be embedded in K, then, for a choice of *t*/*f* edges in D, we have an embedding of each clause gadget of Q_2 in K. In particular, we can always map a literal in each clause of Q_2 to D, ensuring that φ is satisfied. As this is true for any knowledge base K obtained for all possible *t*/*f* assignments to $\{x_i\}$, we obtain Φ is satisfiable.

We note that this result can be extended to alphabets of constant size by encoding x_i as $\hat{x}_i = \lozenge^{i-1}\blacklozenge\lozenge^{n-i-1} \in \{\lozenge, \blacklozenge\}^n$ and y_i as $\hat{y}_i = \vartriangle^{i-1}\blacktriangle\vartriangle^{\ell-i-1} \in \{\vartriangle, \blacktriangle\}^\ell$. $\square$

On the other hand, even if we now allow arbitrary CRPQs on the left, containment remains in Π_2^p.

Theorem 4.4. *Containment of* CRPQ *in* CRPQ(a) *is* Π_2^p*-complete.*

Proof. The lower bound is immediate from Theorem 4.3. For the upper bound, we provide a Σ_2^p algorithm for non-containment, which yields the result. Let $Q_1 \in$ CRPQ, $Q_2 \in$ CRPQ(a), and $\#$ be a symbol not appearing in Q_1 or Q_2. For every atom $A = xRy$ of Q_1 we guess words u_A and v_A of length $\leq |Q_2|$ such that $u_A\Sigma^*v_A \cap L(R) \neq \emptyset$ and $|u_Av_A| < 2|Q_2|$ implies that $u_Av_A \in L(R)$. We guess a component Q_2' of Q_2 and we check that

(1) Q'_2 cannot be embedded in Q'_1, where Q'_1 is the KB resulting from replacing each atom $A = xRy$ with the path $u_A \cdot s_\# \cdot v_A$, where $s_\# = \varepsilon$ if $|u_A v_A| < 2|Q_2|$ and $s_\# = \#$ otherwise; and
(2) for every atom $A = xRy$ of Q_1 such that $|u_A v_A| = 2|Q_2|$ there is $w \in u_A\Sigma^* v_A \cap L(R)$ such that Q'_2 cannot be embedded in w. This last test amounts to checking that either (i) Q'_2 is not homomorphically equivalent to a path or, otherwise, (ii) if Q'_2 is homomorphically equivalent to a path with label $\hat{w}$, we test $u_A\Sigma^* v_A \cap L(R) \cap (\Sigma^*\hat{w}\Sigma^*)^c \neq \emptyset$.

If tests (1) and (2) succeed, we found a knowledge base into which Q_1 can be embedded, but not Q_2. Testing whether Q'_2 can be homomorphically embedded in Q'_1 is in NP as the size of Q'_1 is polynomial in Q_1 and Q_2. Test (2) is in coNP as we need to check for an embedding of Q'_2 for each atom of Q_1. □

Allowing disjunctions in the right query is rather harmless if we only need to consider polynomial-size canonical models to decide containment correctly. Even if such canonical models may become exponentially large, they can sometimes be encoded using polynomial size, allowing for Π^p_2 containment algorithms (cf. Corollary 5.2, Theorem 7.1). However, if we have arbitrary queries on the left, these techniques do not work anymore, to the extent that the problem becomes PSPACE-complete.

The following theorem can be regarded as a generalization of the result of Björklund, Martens, and Schwentick (2013) [Theorem 9] stating that the inclusion problem between a DFA over an alphabet $\Sigma = \{a, b, c\}$ and a regular expressions of the form $\Sigma^* a \Sigma^n b \Sigma^*$ is PSPACE-complete.

Theorem 4.5. *Containment of* CRPQ *in* CRPQ(A) *is* PSPACE*-complete, even if the size of the alphabet is fixed.*

Proof. The upper bound follows from Theorem 5.5, which we prove later. For the lower bound we reduce from the corridor tiling problem, a well-known PSPACE-complete problem (Chlebus 1986). An instance of this problem is a tuple $(T, H, V, \bar{i}, \bar{f}, n)$, where T is the set of tiles, $H, V \subseteq T \times T$ are the horizontal and vertical constraints, encoding which tiles are allowed to occur next to each other and on top of each other, respectively, $\bar{i} = i_1 \dots i_n \in T^n$ is the initial row, $\bar{f} = f_1 \dots f_n \in T^n$ is the final row, and n encodes the length of each row in unary. The question is whether there exists a tiling solution, that is, an $N \in \mathbb{N}$ and a function $\tau : \{1, \dots, N\} \times \{1, \dots, n\} \to T$ such that $\tau(1, 1) \cdots \tau(1, n) = \bar{i}$, $\tau(N, 1) \cdots \tau(N, n) = \bar{f}$ and all horizontal and vertical constraints are satisfied: $(\tau(i, j), \tau(i, j+1)) \in H$ and $(\tau(i, j), \tau(i+1, j)) \in V$ for every i, j in range.

The coding idea is that the query Q_1 is a string describing all tilings with correct start and end tiles, with no horizontal errors, and having rows of the correct length. The query Q_2 describes vertical errors. Then we have $Q_1 \subseteq Q_2$ if and only if there exists no valid tiling, i.e., every tiling has an error.

Let $(T, H, V, \bar{i}, \bar{f}, n)$ be a corridor tiling instance as defined before. From the original proof of Chlebus (1986), it follows that the following restricted version of corridor tiling remains PSPACE-complete. The set of tiles T is partitioned into $T = T_1 \uplus T_2 \uplus T_3$, such that each row in a solution must belong to $T_1^* T_2 T_1^* \cup T_1^* T_3 T_3 T_1^*$. The original proof furthermore implies, that (i) $(T_1 \times T_1) \cup (T_1 \times T_2) \cup (T_2 \times T_1) \subseteq H$; and (ii) for all $u, v \in T_3$ with $(u, v) \in H$ we have that $T_1 \times \{u\} \subseteq H$ and $\{v\} \times T_1 \subseteq H$. This implies that our horizontal errors can only occur with T_2 or T_3 involved, so only once per row. Therefore, we construct a new set $\tilde{H}$ defined as follows: $\tilde{H} = H \cap (T_2 \times T_1 \cup T_1 \times T_2 \cup T_3 \times T_3)$. This set is used in the definition of query Q_1.

We encode tiles as follows: each tile t_i has an encoding $\widehat{t_i}$ given by $\triangle^{i-1} \blacklozenge \triangle^{|T|-i-1} e_1 \cdots e_{|T|}$, where $e_j = \blacktriangle$ if $(t_i, t_j) \in V$ and $e_j = \triangle$, otherwise. The second half of the encoding of a tile describes which tiles are allowed to occur above the tile. The query Q_1 is

$$\widehat{i_1} \cdots \widehat{i_n} \left(\sum_{i=0}^{n-2} \sum_{(v_1, v_2) \in \tilde{H}} (\widehat{T_1})^i \widehat{v_1} \widehat{v_2} (\widehat{T_1})^{n-i-2} \right)^* \widehat{f_1} \cdots \widehat{f_n} \, .$$

We note that Q_1 encodes exactly the tilings without horizontal errors, due to the imposed restrictions.

The query Q_2 is $\triangle(\triangle + \blacktriangle + \triangle + \blacklozenge)^{(2n-1)|T|-1} \blacklozenge$ and matches exactly those positions where a vertical error occurs, exploiting the encoding of vertical constraints in the second half of each tile's encoding. □

5 Simple Transitive Closures

In this section, we investigate what happens if we consider fragments that only allow singleton transitive closures, that is, transitive closures of single symbols. Our first results imply a number of Π^p_2-results in Table 2.

Theorem 5.1. *Containment of* CRPQ(a, a^*) *in* CRPQ(a) *is* Π^p_2*-hard, even if the size of the alphabet is fixed.*

Proof sketch. We use a similar reduction as in Theorem 4.3. The only change we make is that we replace the expressions $t + f$ in Q_1 with $t^* f$-paths. Intuitively, Q_1 sets a variable x_i to true if and only if there exists at least one t-edge after the x_i-edge. The query Q_2 is not changed. □

Corollary 5.2. *Containment of* CRPQ(A, a^*) *in* CRPQ *is in* Π^p_2.

Proof. This will be a corollary of Theorem 7.1, since CRPQ(A, a^*) is a fragment of CRPQ(W). □

On the other hand, if we allow arbitrary queries on the left and simple transitive closure on the right-hand query, the problem becomes PSPACE-hard.

Theorem 5.3. *Containment of* CRPQ *in* CRPQ(a, a^*) *is* PSPACE*-complete, even if the size of the alphabet is fixed.*

Proof sketch. We adapt the encoding in the proof of Theorem 4.5, by (a) replacing each symbol $\sigma \in \{\lozenge, \blacklozenge, \triangle, \blacktriangle\}$ with $\sigma\$$, where $\$$ is a new symbol, and (b) replacing Q_2 with $\triangle\$(\lozenge^* \blacklozenge^* \triangle^* \blacktriangle^* \$)^{(2K-1)|T|-1} \blacklozenge\$$. □

Interestingly, the complexity of containment can drop by adding distinguished variables to the query:

Proposition 5.4. *The complexity of Containment of (1)* CRPQ *in* CRPQ(A) *and (2)* CRPQ *in* CRPQ(a, a^*) *is in* Π_2^p *if every component of each query contains at least one distinguished variable.*

Finally we show that, as long as the right query only has single symbols under Kleene closures, query containment remains PSPACE-complete.

Theorem 5.5. *Containment of* CRPQ *in* CRPQ(A, a^*) *is* PSPACE*-complete.*

Proof. The lower bound is immediate from Theorem 4.5. For the upper bound we provide a PSPACE-algorithm for non-containment. Let $Q_1 \in$ CRPQ, $Q_2 \in$ CRPQ(A, a^*), and # be a symbol not appearing in Q_1 and Q_2. We first note that each component of Q_2 can express at most $|Q_2|$ many label changes on a path. Hence it suffices if the algorithm stores just the part of a path that corresponds to the last $|Q_2|$ label changes. Furthermore, a standard pumping argument yields that, in a counterexample, the length of segments that only use a single label can be limited to $|Q_1| + |Q_2|$.

Therefore, for each atom of $A = xRy$ of Q_1, the PSPACE-algorithm guesses words u_A, v_A of length at most $|Q_2| \times (|Q_1| + |Q_2|)$, such that $u_A\Sigma^*v_A \cap L(R) \neq \emptyset$ and, if u_A or v_A has less than $|Q_2|$ label changes, then $u_Av_A \in L$. We guess a component of Q_2' and check that

(1) Q_2' cannot be embedded in Q_1', where Q_1' is the KB resulting from replacing each atom $A = xRy$ with the path $u_A \cdot s_\# \cdot v_A$, where $s_\# = \varepsilon$ if u_A or v_A contains less than $|Q_2|$ label changes and $s_\# = \#$ otherwise; and

(2) for every atom $A = xRy$ of Q_1 such that u_A and v_A have $|Q_2|$ label changes there is $w \in u_A\Sigma^*v_A \cap L(R)$ such that Q_2' cannot be embedded in w.

If tests (1) and (2) succeed, we found a knowledge base into which Q_1 can be embedded, but Q_2 cannot. Test (1) is in coNP as Q_1' has size polynomial in Q_1 and Q_2. Test (2) is in polynomial space, as the restricted language of Q_2 allows us to guess and verify the existence of w on the fly while only keeping the path corresponding to the last $|Q_2|$ label changes in memory with length at most $|Q_2| \times (|Q_1| + |Q_2|)$. □

6 Transitive Closures of Sets

In this section we show that adding just a little more expressiveness makes containment EXPSPACE-complete. This high complexity may be surprising, considering that it already holds for CRPQ(a, A^*) queries, which is a fragment that merely extends ordinary conjunctive queries *by adding transitive reflexive closures of simple disjunctions*. Our proof is inspired by the hardness proof in (Calvanese et al. 2000) for general CRPQs, but we need to add a number of non-trivial new ideas to make it work for CRPQ(a, A^*).

Disjunction creation. A significant restriction that is imposed on CRPQ(a, A^*) is that the non-transitive atoms are not allowed to have disjunctions in their expressions. We get around this by the following idea that generates disjunctive *bad patterns* out of conjunctions — we use a similar idea in our next proof.

Consider the following query Q_2 where ℓ is a special helper symbol, $y_1\ \ell^* \cdot s_1 \cdot \ell \cdot s_2 \cdot \ell^* y_2$. For query Q_1 given by $\bigwedge_{\sigma \in \Sigma \setminus \{\ell\}} x_1 \sigma x_1 \wedge x_1 \ell\ (\Sigma \setminus \{\ell\})^*\ \ell x_2 \wedge \bigwedge_{\sigma \in \Sigma \setminus \{\ell\}} x_2 \sigma x_2$ it is clear that Q_1 allows for exactly two ℓ, and hence, if Q_1 were be contained in Q_2, one of the patterns s_1 or s_2 has to be be matched to the $(\Sigma \setminus \{\ell\})^*$ fragment in the middle. Essentially, we capture all bad patterns matching either s_1 or s_2, thereby "creating" the result of a disjunction.

Theorem 6.1. *Containment of* CRPQ(a, A^*) *in* CRPQ(a, A^*) *is* EXPSPACE*-hard, even if the size of the alphabet is fixed.*

Proof sketch. We reduce from the exponential width corridor tiling problem. That is, we have

- a finite set $T = \{t_1, \dots, t_m\}$ of tiles,
- initial and final tiles $t_I, t_F \in T$, respectively,
- horizontal and vertical constraints $H, V \subseteq T \times T$,
- a number $n \in \mathbb{N}$ (in unary),

and we want to check if there is a $k \in \mathbb{N}$ and a tiling function $\tau\colon \{1, \dots, k\} \times \{1, \dots, 2^n\} \to T$ such that $\tau(1, 1) = t_I$, $\tau(k, 2^n) = t_F$, and all horizontal and vertical constraints are satisfied. In order to have a fixed alphabet, we encode tiles from T as words from $\{\lozenge, \blacklozenge\}^m$. The i-th tile t_i is encoded as $\hat{t}_i = \lozenge^{i-1}\blacklozenge\lozenge^{m-i-1} \in \{\lozenge, \blacklozenge\}^m$.

A tiling τ is encoded as a string over the alphabet $\mathbb{B} = \{\$, 0, 1, \lozenge, \blacklozenge, \#\}$, where \$ is the row separator, 0 and 1 are used to encode addresses for each row of the tiling from 0 to $2^n - 1$ as binary numbers, # separates the individual bits of an address, and $\lozenge$ and $\blacklozenge$ are used to encode the individual tiles. We visualize a tiling as a matrix with k rows of 2^n tiles each. An example of a tiling τ with $n = 3$ is below:

$$\begin{array}{lccr}
\widehat{\tau(k,1)}0\#0\#0\widehat{\tau(k,2)}0\#0\#1 & \cdots & \widehat{\tau(k,2^3)}1\#1\#1 & \$ \\
\qquad\qquad\vdots & \iddots & \vdots & \vdots \\
\$\,\widehat{\tau(1,1)}0\#0\#0\widehat{\tau(1,2)}0\#0\#1 & \cdots & \widehat{\tau(1,2^3)}1\#1\#1 & \$
\end{array}$$

The queries Q_1 and Q_2 use the alphabet $\mathbb{A} = \mathbb{B} \cup \{[,], \langle, \rangle, b, \star\}$. This new set contains helper symbols [and] which we use for disjunction creation (in a similar way as we explained before the Theorem statement), and $\langle$ and $\rangle$ denote the start and end of the tiling. The b-symbol is used for a special edge that we use for checking vertical errors. Query Q_1 is given in Figure 4 and query Q_2 is sketched in Figure 5. For convenience we use $\mathbb{B}_{\langle\rangle}$ to abbreviate $\mathbb{B} \cup \{\langle, \rangle\}$, $\mathbb{B}_{[]\langle\rangle}$ to abbreviate $\mathbb{B}_{\langle\rangle} \cup \{[,]\}$, and $\mathbb{B}_{\overline{\$}}$ to abbreviate $\mathbb{B} \setminus \{\$\}$.

The intuition is that the tiling is encoded in the $\mathbb{B}^*$-edge of Q_1, i.e. the only edge that is labeled by a language that is not a single symbol. The query Q_2 consists of a sequence of *bad patterns*, one for each possible kind of violation of the described encoding or the horizontal and vertical constraints. The queries are designed in such a way that Q_2 cannot be embedded if a valid tiling is encoded in a canonical model of Q_1. Otherwise, at least one of the bad patterns can be embedded in the encoding of the tiling. The other bad patterns can be embedded at the nodes z_2 and z_7 of Q_1, as these nodes have one self loop for every symbol of the alphabet except $\star$.

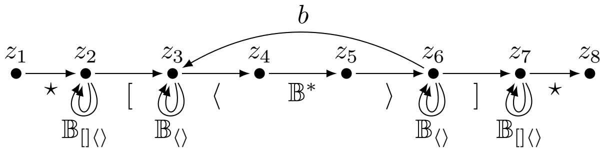

b
z_1
z_2
z_3
z_4
z_5
z_6
z_7
z_8
$\star$
$[$
$\langle$
$\mathbb{B}^*$
$\rangle$
$]$
$\star$
$\mathbb{B}_{[]\langle\rangle}$
$\mathbb{B}_{\langle\rangle}$
$\mathbb{B}_{\langle\rangle}$
$\mathbb{B}_{[]\langle\rangle}$

Figure 4: Query Q_1 in the proof of Theorem 6.1. Double-self-loops indicate a distinct self-loop for every single symbol, i.e., not a self-loop labeled with the alphabet.

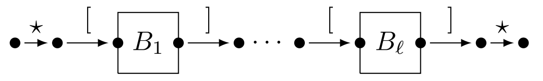


Figure 5: Query Q_2 in the proof of Theorem 6.1. The B_i denote "bad patterns" described in the proof; each B_i has a 'left' and 'right' distinguished variable as in the picture.

We can easily design (sets of) patterns, where each pattern is a simple path, to catch the following errors: malformed encoding of a tile, malformed encoding of an address, non-incrementing addresses, missing initial or final \$, wrong initial or final tile, and an error in the horizontal constraints.

The most difficult condition to test is an error in the vertical constraints, which we encode with the pattern $G^{t,t'}$ for every $(t,t') \notin V$, given by

$$\bigwedge_{1\le i\le n} G_i^{t,t'} \wedge \bigwedge_{\substack{i,j\in\{1,\dots,n\}\\ c,d\in\{0,1\};|i-j|=1}} (x_{i,c}^{t,t'} L x_{j,d}^{t,t'} \wedge y_{i,c}^{t,t'} L y_{j,d}^{t,t'}) ,$$

where $G_i^{t,t'}$ is given in Figure 6 and $L = b^*\mathbb{B}^*_{\langle\rangle}b^*$. We first explain the intuition behind $G_i^{t,t'}$. We assume that the vertical error occurs at tile t having 0 as i-th bit of its address. In that case, the variable $x_{i,0}^{t,t'}$ should be embedded just before the encoding of t, while $y_{i,0}^{t,t'}$ should be embedded in the next row just after the tile t' with the same i-th bit. This is enforced as there is one \$ between $x_{i,0}^{t,t'}$ and $y_{i,0}^{t,t'}$, ensuring that both variables occur in consecutive rows. The variables $x_{i,1}^{t,t'}$ and $y_{i,1}^{t,t'}$ are simply embedded at the node corresponding to z_6 of Q_1.

In the case that the i-th bit is 1, we embed $x_{i,0}^{t,t'}$ and $y_{i,0}^{t,t'}$ at z_3, while $x_{i,1}^{t,t'}$ and $y_{i,1}^{t,t'}$ are embedded at the tiles violating the vertical constraint, as described in the previous case.

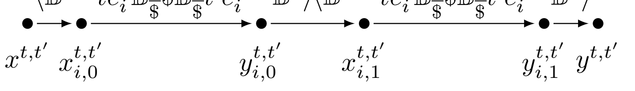

$\langle\mathbb{B}^*$
$\widehat{t}e_i^0\mathbb{B}^*_{\overline{\$}}\$\mathbb{B}^*_{\overline{\$}}\widehat{t'}e_i^0$
$\mathbb{B}^*\rangle\langle\mathbb{B}^*$
$\widehat{t}e_i^1\mathbb{B}^*_{\overline{\$}}\$\mathbb{B}^*_{\overline{\$}}\widehat{t'}e_i^1$
$\mathbb{B}^*\rangle$
$x^{t,t'}$
$x_{i,0}^{t,t'}$
$y_{i,0}^{t,t'}$
$x_{i,1}^{t,t'}$
$y_{i,1}^{t,t'}$
$y^{t,t'}$

Figure 6: Subquery $G_i^{t,t'}$ in the proof of Theorem 6.1. Here, $e_i^a = (\{0,1\}^*\#)^{i-1}a(\#\{0,1\}^*)^{n-i-1}$ is the language enforcing the i-th bit to be a.

Altogether, $G_i^{t,t'}$ verifies that there are positions v and w in consecutive rows of the encoding such that the tiles adjacent to v and w would violate the vertical constraints and the positions agree on the i-th bit of the address. To ensure that the positions v and w agree on *all* n bits of the address we have to ensure that the n patterns $G_1^{t,t'},\dots,G_n^{t,t'}$ all refer to the *same* two positions in the tiling. This is why we have the additional conjuncts with language $L = b^*\mathbb{B}^*_{\langle\rangle}b^*$ in $G^{t,t'}$. The language L is chosen to ensure that there exists exactly one node v in the tiling such that all the variables $x_{1,j}^{t,t'},\dots,x_{n,j}^{t,t'}$, for $j \in \{0,1\}$ are either embedded at v, at the node corresponding to z_3 from Q_1, or at the node corresponding to z_6 from Q_1. If there were two variables $x_{i,c}^{t,t'}$ and $x_{j,d}^{t,t'}$ embedded at different positions between z_3 and z_6 then there is a k and $\tilde{c},\tilde{d}$ such that $x_{k,\tilde{c}}^{t,t'}$ and $x_{k+1,\tilde{d}}^{t,t'}$ are embedded at different positions and thus at least one of the conjuncts $x_{k,\tilde{c}}^{t,t'}Lx_{k+1,\tilde{d}}^{t,t'}$ and $x_{k+1,\tilde{d}}^{t,t'}Lx_{k,\tilde{c}}^{t,t'}$ has to be violated, as the symbol b can be read only at the beginning or end of a string in L (recall that $b \notin \mathbb{B}_{\langle\rangle}$). The argument for the y-variables and the position w is analogous.

To conclude, whenever there exists a valid tiling, we have a canonical knowledge base with the encoding of a tiling occurring between z_4 and z_5. To embed Q_2 into this, we need to span the full length flanked by the $\star$'s in the start and the end. Thanks to (i) the symbols $[,]$ flanking the bad patterns B_i in Q_2, and (ii) the presence of these symbols only at edges from nodes z_2, z_7 in Q_1, at least one of the bad patterns must embed into the part between z_3 and z_6. If there is no error, we cannot embed Q_2, and hence no B_i can be mapped between z_3 and z_6 and we have $Q_1 \not\subseteq Q_2$. On the other hand, when there is no valid tiling, for each canonical knowledge base with a 'guessed' tiling, Q_2 maps one of the B_i between z_3 and z_6, and can hence embed completely from $\star$ to $\star$, giving $Q_1 \subseteq Q_2$. ☐

Remark 6.2. *We observe that the queries Q_1 and Q_2 in Theorem 6.1 have bounded treewidth. Treewidth is a commonly used parameter in parameterized complexity analysis and intuitively, captures how close the graph is to a tree. A tree has treewidth 1, while K_n, the complete graph on n vertices has treewidth $n-1$. It is known that the containment problem of CQs with bounded treewidth (as is the evaluation problem of CQs with bounded treewidth) is in* PTIME *(Chekuri and Rajaraman 2000). In this light, it is surprising how the complexity of containment increases to* EXPSPACE *already for* CRPQ(a, A^*)*,* even for queries of bounded treewidth.

7 Deutsch and Tannen's W-Fragment

The complexity of containment of CRPQs with restricted regular expressions has also been investigated by Deutsch and Tannen (2002). Their work was motivated by the types of restrictions imposed on navigational expressions in the query language XPath. Interestingly, they left some questions open, such as the complexity of containment for CRPQs using expressions from their *W-fragment*.[3] The W-

[3]The nomenclature of this fragment is a mystery to us. Even Deutsch and Tannen say: "The fragments called W and Z have

fragment is defined by the following grammar:

$$\begin{array}{lcl} R & \rightarrow & \sigma \mid \_ \mid S^* \mid R \cdot R \mid (R + R) \\ S & \rightarrow & \sigma \mid \_ \mid S \cdot S \end{array}$$

Here, $\sigma \in \Sigma$ and $\_$ is a wildcard, i.e., it matches a single, arbitrary symbol from the infinite set Σ. In the RPQs underlying Table 1, wildcards occurred in 0% (40 out of 55M) property paths in Wikidata queries, but in ~4.30% of the property paths in valid and in 15.68% of the property paths in unique DBpedia$^{\pm}$ queries. By CRPQ(W), we denote CRPQs where the regular expressions are from the W-fragment.

Deutsch and Tannen (2002) claimed that containment for CRPQ(W) is PSPACE-hard, but their proof, given in Appendix C of their article, has a minor error: it uses the assumption that Σ, the set of edge labels, is finite. In fact, we show that containment of CRPQ(W) queries is in Π_2^p. Furthermore, the right query can even be relaxed completely.

Theorem 7.1. *Containment of* CRPQ(W) *in* CRPQ *is in* Π_2^p.

Proof. Let $Q_1 \in$ CRPQ(W) and $Q_2 \in$ CRPQ. We first show a small model property. More precisely, we show that whenever there is a counterexample to the containment, then there also exists a canonical model B of Q_1 such that $B \notin Q_2$ and B can be represented by a polynomial size graph where each edge is either labeled with a single symbol or by w^i, where w is of size linear in Q_1 and i is at most $2^{|Q_2|^3}$.

Assume that B is the smallest graph that is a canonical model of Q_1 and has no satisfying homomorphism from Q_2. W.l.o.g., we assume that all occurrences of $\_$ in Q_1 are replaced by the same symbol \$ that does not occur in Q_2. As the W-fragments allows only a fixed string below every star, every path of B can be written as $w_0^{\ell_0} a_1 w_1^{\ell_1} a_2 \cdots a_n w_n^{\ell_n}$, where $n < |Q_1|$ and $\ell_i \in \mathbb{N}$, as all long segments of a path have to result from applying the Kleene star to a fixed string.

It remains to show that for every path, all multiplicities are at most $2^{|Q_2|^3}$. We assume towards a contradiction that there exists a path p in B, where for some string w, the multiplicity ℓ is larger than $2^{|Q_2|^3}$. We assume w.l.o.g. that all NFAs in Q_2 share the same transition function δ over the same set of states P, which can be achieved by taking the disjoint union of all sets of states. Let M be the adjacency matrix of the transition relation for the string w, i.e., M is a Boolean $|P| \times |P|$ matrix, that has a 1 on position (i, i'), if and only if $\delta^*(q_i, w) = q_{i'}$. By the pigeonhole principle, there have to be j and k such that $0 \leq j < k \leq 2^{|P|^2}$ and $M^j = M^k$. We now shorten p by $k - j$ copies of w and call the resulting graph B'. It is obvious that Q_1 can still embed into B'. We have to show that Q_2 cannot embed into B'. Towards a contradiction we assume that h is a satisfying homomorphism from Q_2 to B'. Let p' be a subpath of the path p that spans at least j copies of w such that no node of p' occurs in the image of h. Such a subpath exists due to the length of p still being at least $2^{|P|} + j$ and the fact that the sizes of $|P|$ and the image of h are both bounded by $|Q_2|$. We now insert $k - j$ copies of w into p'. By definition of M and the fact that $M^j = M^k$, we have that h is also a satisfying homomorphism from Q_2 to B, the desired contradiction.

We note that the minimal model property implies that the smallest counter examples can be stored using only polynomial space by storing the multiplicities of strings in binary. The Π_2^p-algorithm universally guesses such a polynomial size representation of a canonical model B of Q_1. Then it tests whether there exists an homomorphism from Q_2 into B by guessing an embedding. Testing whether a guessed mapping is indeed a satisfying homomorphism can be done in polynomial time using a square-and-multiply algorithm to compute any necessary $\delta^*(q, w^i)$. $\square$

technical importance but their definitions did not suggest anything better than choosing these arbitrary names."

Next we show that, if we assume a *finite* set of edge labels Γ for knowledge graphs, the containment problem of CRPQ(W) is not just PSPACE-hard (as Deutsch and Tannen showed), but even EXPSPACE-complete. The important technical difference with Theorem 7.1 is that, when the labeling alphabet Γ is finite, it is not always possible to replace occurrences of the wildcard $\_$ with a fresh symbol that doesn't appear in either query. Therefore, the counterexamples cannot be stored in a compact way. Even though this is a different setting than all the other results in the paper, we provide a proof, because the problem was left open by Deutsch and Tannen (2002).

Proposition 7.2. *If edge labels of knowledge bases come from a finite alphabet* Γ*, then containment of* CRPQ(W) *in* CRPQ(W) *is* EXPSPACE*-complete.*

Proof. To avoid confusion with an infinite alphabet, we write Γ instead of $\_$. We change the languages used in the proof of Theorem 6.1. We apply the following homomorphism h to all single label languages of Q_1 and Q_2 (including the languages resulting from the double-self-loops in Figure 4): $\# \mapsto \varepsilon$, $\$ \mapsto \$\triangle\blacktriangle$, $\sigma \mapsto \sigma\blacktriangle\blacktriangle$ for $\sigma \in \mathbb{B} \setminus \{\$, \#\}$, and $\sigma \mapsto \sigma\triangle\triangle \in \mathbb{A} \setminus \mathbb{B}$, where $\blacktriangle$ and $\triangle$ are new symbols, i.e., we encode every symbol σ of our original construction by the three symbols $\sigma\sigma_1\sigma_2$, where $\sigma_1, \sigma_2 \in \{\blacktriangle, \triangle\}$ encode whether σ belongs to $\mathbb{B}$ and $\mathbb{B}_{\overline{\$}}$, respectively.

We replace every occurrence of $\mathbb{B}^*$ with the language $(\Gamma\Gamma\blacktriangle)^*$ and every occurrence of $\mathbb{B}_{\overline{\$}}^*$ with the language $(\Gamma\blacktriangle\blacktriangle)^*$. We replace e_i^a as used in Figure 6 with $((0+1)\blacktriangle\blacktriangle)^{i-1} a \blacktriangle\blacktriangle((0+1)\blacktriangle\blacktriangle)^{n-i-1}$.

The last change is that we add further bad patterns to the construction of Q_2 that detects whenever the language $(\Gamma\Gamma\blacktriangle)^*$ resulting from the $\mathbb{B}^*$ in Q_1 produces an invalid pattern, i.e., a triple that is not in the image of h. $\square$

8 Related Work

The most relevant work to us is that of Calvanese et al. (2000), who proved that containment for conjunctive regular path queries, with or without inverses, is EXPSPACE-complete, generalizing the EXPSPACE upper bound for CRPQs of Florescu, Levy, and Suciu (1998).

Deutsch and Tannen (2002) have also studied the containment problem for CRPQ with restricted classes of regular expressions. They chose fragments of regular expressions based on expressions in query languages for XML, such as StruQL, XML-QL, and XPath. The fragments they propose are orthogonal to the ones we study here. This is because they allow wildcards and union of words as long as they are not under a Kleene star, while we disallow wildcards and allow union of letters under Kleene star. Concretely, they allow $(aa + b)$, which we forbid. On the other hand, their fragments $(*, l^*, |)$ and W do not allow unions under Kleene star, i.e., they cannot express $(a + b)^*$. Their fragments Z and full CRPQs allow unions under Kleene star, but are already EXPSPACE-complete.

Florescu, Levy, and Suciu (1998) studied a fragment of conjunctive regular path queries with wildcards for which the containment problem is NP-complete—thus, it has the same complexity as containment for conjunctive queries. In their fragment, they only allow single symbols, transitive closure over wildcards, and concatenations thereof.

Miklau and Suciu (2004) were the first to investigate containment and satisfiability of *tree pattern queries*, which are acyclic versions of the CRPQs studied by Florescu, Levy, and Suciu (1998). Tree pattern queries are primarily considered on tree-structured data, but the complexity of their containment remains the same if one allows graph-structured data (Miklau and Suciu 2004; Czerwiński et al. 2018). Containment of tree pattern queries was considered in various forms in (Miklau and Suciu 2004; Neven and Schwentick 2006; Wood 2003; Czerwiński et al. 2015).

Björklund, Martens, and Schwentick (2011) studied containment of conjunctive queries over tree-structured data and and proved a trichotomy, classifying the problems as in PTIME, CONP-complete, or Π_2^p-complete. Their results cannot be lifted to general graphs since they use that, if a child has two direct ancestors, then they must be identical.

Sagiv and Yannakakis (1980) studied the equivalence and therefore the containment problem of relational expressions with query optimization in mind. They show that when select, project, join, and union operators are allowed, containment is Π_2^p-complete.

Chekuri and Rajaraman (2000) showed that containment of conjunctive queries is in PTIME when the right-hand side has bounded treewidth. More precisely, they give an algorithm that runs in $(|Q_1| + |Q_2|)^k$, where k is the width of Q_2. So their algorithm especially works for acyclic queries.

Calvanese et al. (2001) provide a PSPACE-algorithm for containment of tree-shaped CRPQs with inverses. The algorithm also works if only the right-hand side is tree-shaped. Figueira (2020) shows that containment of UC2RPQs is in PSPACE if the class of graphs considered has "bounded bridgewidth" (= size of minimal edge separator is bounded) and is EXPSPACE-complete otherwise. Barceló, Figueira, and Romero (2019) studied the boundedness problem of UC2RPQs and prove that its EXPSPACE-completeness already holds for CRPQs. (A UC2RPQ is bounded if it is equivalent to a union of conjunctive queries.)

The practical study of (Bonifati, Martens, and Timm 2019) that we mentioned in the beginning of the paper and that was crucial for the motivation of this work would not have been possible without the efforts of the Dresden group on Knowledge-Based Systems (Malyshev et al. 2018), who made sure that anonymized query logs from Wikidata could be released. Bonifati, Martens, and Timm (2019) studied the same log files as Bielefeldt, Gonsior, and Krötzsch (2018).

It should be noted that several extensions and variants of CRPQs have been studied in the literature. Notable examples are nested regular expressions (Pérez, Arenas, and Gutierrez 2010), CRPQs with node- and edge-variables (Barceló, Libkin, and Reutter 2014), regular queries (Reutter, Romero, and Vardi 2015), and GXPath (Libkin, Martens, and Vrgoč 2016).

9 Conclusions and Further Work

We have provided an overview of the complexity of CRPQ containment in the case where the regular expressions in queries come from restricted, yet widely used classes in practice. A first main result is that, even when the regular expressions are from the restricted class CRPQ(a, A^*), the containment problem remains EXPSPACE-hard. Second, in the case that transitive closures are only allowed over single symbols, the complexity of CRPQ containment drops significantly. This is rather good news in practice, because, as we see in Table 2, the types of CRPQs for which containment falls into such lower complexities are extremely common.

Contrary to the EXPSPACE lower bound reduction of Calvanese et al. (2000), the shape of queries (i.e., its underlying graph) is quite involved, and it crucially involves cycles. This immediately raises a number of questions.

- What is the complexity of Containment of CRPQ(a, A^*) in CRPQ(a, A^*) if one of the sides is only a path or a DAG?
- If one takes a careful look at our results, we actually settle the complexity of all forms of containment $\mathcal{F}_1 \subseteq \mathcal{F}_2$ where $\mathcal{F}_i$ is one of our considered classes, except the cases of Containment of CRPQ(a, A^*) in CRPQ(A) and Containment of CRPQ(a, A^*) in CRPQ(a, a^*). What is the complexity in these cases?

Of course, it would be interesting to understand which of our results can be extended towards C2RPQs, which would slightly increase the coverage of the queries we consider in Table 2. We believe that all our upper bounds can be extended and we plan to incorporate these results in an extended version of the paper.

Another direction could be to combine our fragments with arithmetic constraints. There is a lot of work done considering query containment of conjunctive queries with arithmetic constraints (which is Π_2^p-complete), see for example Afrati (2019) and the related work mentioned there. We would like to understand to which extent such constraints can be incorporated without increasing the complexity of containment.

It would also be interesting to investigate the problem of *boundedness* (Barceló, Figueira, and Romero 2019) for the studied classes of CRPQ; understanding whether a query is 'local' might be of interest for the graph exploration during its evaluation.

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