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Teaching an RDBMS about ontological constraints

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ABSTRACT
In the presence of an ontology, query answers must reflect not only data explicitly present in the database, but also implicit data, which holds due to the ontology, even though it is not present in the database. A large and useful set of ontology languages enjoys FOL reducibility of query answering: answering a query can be reduced to evaluating a certain first-order logic (FOL) formula (obtained from the query and ontology) against only the explicit facts.

We present a novel query optimization framework for ontology-based data access settings enjoying FOL reducibility. Our framework is based on searching within a set of alternative equivalent FOL queries, i.e., FOL reformulations, one with minimal evaluation cost when evaluated through a relational database system. We apply this framework to the DL-LiteR Description Logic underpinning the W3C’s OWL2 QL ontology language, and demonstrate through experiments its performance benefits when two leading SQL systems, one open-source and one commercial, are used for evaluating the FOL query reformulations.

1. INTRODUCTION
Ontology-based data access (OBDA, in short) [22] aims at exploiting a database, i.e., facts, on which hold ontological constraints, i.e., deductive constraints modeling the application domain under consideration. For instance, an ontology may specify that any author is a human, has a name, and must have authored some papers. Ontological constraints may greatly increase the usefulness of a database: for instance, a query asking for all the humans must return all the authors, just because of a constraint stating they are human; one does not need to store a human tuple in the database for each author. The data interpretations enabled by the presence of constraints has made OBDA a technique of choice when modeling complex real-life applications. For instance, in the medical domain, Snomed Clinical Terms is a biomedical ontology providing a comprehensive clinical terminology; the British Department of Health has a roadmap for standardizing medical records across the country, using this ontology etc.

While query answering under constraints is a classical database topic [2], research on OBDA has bloomed recently through many ontology constraints languages, e.g., Datalog+ [12], Description Logics [1] and Existential Rules [8], or RDF Schema for RDF graphs. OBDA query answering is the task of computing the answer to the given query, by taking into account both the facts and the constraints holding on them. In contrast, query evaluation as performed by database servers leads to computing only the answers derived from the data (facts), while ignoring the constraints.

A large and useful class of ontology languages enjoy first-order logic (FOL) reducibility (a.k.a. rewritability) of query answering, e.g., [13][12][25]. Query answering under constraints formulated in these languages reduces to the evaluation of the FOL query reformulation, obtained by compiling the constraints into the query, against the facts alone. Evaluating this FOL query in a relational database management system (RDBMS) by translation into SQL against the facts, suffices to compute the complete query answer.

A longstanding issue in reformulation-based query answering is that FOL reformulations tend to be very complex queries, involving very large unions (sometimes with hundreds or thousands of union terms) and/or numerous redundant subexpressions. Such queries are very different from the typical ones RDBMS optimizers are tuned for, thus RDBMSs perform poorly at evaluating them. To mitigate this issue, OBDA optimization research has mostly focused on producing FOL reformulations where redundancy is avoided as much as possible, e.g., [30, 29, 14, 34, 20, 35, 33, 18].

We present a more general, performance-oriented approach: we propose a query optimization framework for any logical OBDA setting enjoying FOL reducibility of query answering. We extend the language of FOL reformulations beyond those considered so far in the literature, and investigate several (equivalent) FOL reformulations of a given query, out of which we pick one likely to lead to the best evaluation performance. This contrasts with existing works from the semantic query answering literature (cf. Section 7), which use reformulation languages allowing single FOL reformulation (modulo minimization). Considering a set of reformulations and relying on a cost model to pick a most efficient one has a very visible impact on the efficiency and feasibility of query answering: indeed, picking the wrong reformulation may cause the RDBMS simply to fail evaluating it (typically due to very lengthy queries), while in other cases it leads to bad performance.

We apply this framework to the DL-LiteR Description Logic [13] underpinning the popular W3C’s OWL2 QL standard for rich Semantic Web applications. Query answering in DL-LiteR has received significant attention in the literature, notably techniques based on FOL reducibility, e.g., [13][1][30][31][17][24].

Contributions. We bring the following contributions to the problem of optimizing FOL reducible query answering (see Figure 1):
1. For logical formalisms enjoying FOL reducibility of query answering, we provide a general optimization framework that reduces query answering to searching among a set of alternative equivalent FOL reformulations, one with minimal evaluation cost in an RDBMS (Section 3). In Figure 1, from the query q and the set of ontological constraints T, we derive first, a space of query covers, shown in the top white-background box, and denoted C with some subscripts; from each such cover we show how to derive a FOL query that may be a FOL reformulation of q w.r.t. T.
2. We characterize interesting spaces of such alternative equivalent FOL queries for DL-LiteR (Section 4).
First, we identify a sufficient safety condition to pick covers that
for sure lead to FOL reformulations of the query. This condition is met by the covers in the top yellow box in Figure 1 and is not met by $C_{\varphi}$ above them. Our safe cover space allows considering FOL reformulations encompassing those previously studied in the literature. Second, we introduce a set of generalized covers (bottom yellow box in Figure 1) and a generalized cover-based reformulation technique, which always yields FOL query reformulations, oftentimes more efficient than those based on simple covers.

Our approach can be combined with, and helps optimizing, any existing reformulation technique for DL-Lite$_{\mathbb{Q}}$. We then optimize query answering in the setting of DL-Lite$_{\mathbb{Q}}$ by enumerating simple and generalized covers, and picking a cover-derives FOL reformulation with lowest estimated evaluation cost w.r.t. an RDBMS cost model estimation (denoted by the bidirectional $\epsilon$-labeled arrows in the figure). We provide two algorithms, an exhaustive and a heuristic, for this task (Section 5).

Evaluating any of our FOL reformulations through an RDBMS leads (thick arrows at the right of Figure 1) to the query answer reflecting both the data and the constraints. We demonstrate experimentally the effectiveness and the efficiency of our query answering technique for DL-Lite$_{\mathbb{Q}}$, by deploying our query answering technique on top of Postgres and DB2, using several alternative data layouts (Section 6).

From a query processing and optimization perspective, our approach can be seen as belonging to the so-called strategic optimization stage introduced in [24] (where application semantics is injected into the query); it is also similar in spirit to the syntax-level rewrites performed by optimizers such as Oracle 10g’s [6]. We share with [24] the idea of injecting semantics first, and like [6], we use cost estimation to guide our rewrites; a common theme is to rewrite before ordering joins, selecting physical operators etc. From this angle, our contribution can be seen as a set of alternatives (rewritings) with correctness guarantees and algorithms to guide such rewritings, for the special class of queries obtained from FOL reformulations of QG against ontologies.

In the sequel, Section 2 recalls preliminary notions on knowledge bases and DL-Lite$_{\mathbb{Q}}$. Then, we detail the above contributions. Finally, we discuss related work and conclude in Section 7.

### 2. PRELIMINARIES

We introduce knowledge bases (Section 2.1), queries and query answering (Section 2.2), and finally position our work from a query optimization perspective, highlighting the hard issues (Section 2.3).

Table I summarizes the main notations of this work.

#### 2.1 Knowledge bases

As commonly known, a knowledge base (KB) $K$ consists of a TBox $T$ (ontology, or axiom set) and an ABox $A$ (database, or fact set), denoted $K = (T, A)$, with $T$ expressing constraints on $A$. Most popular Description Logic dialects [4], and in particular DL-Lite$_{\mathbb{Q}}$ [13], build $T$ and $A$ from a set $NC$ of concept names (unary predicates), a set $NR$ of role names (binary predicates), and a set $NI$ of individuals (constants). The ABox consists of a finite number of concept assertions of the form $A(a)$ with $a \in NC$ and $a \in NI$, and of role assertions of the form $R(a, b)$ with $R \in NR$ and $a, b \in NI$. The TBox is a set of axioms, whose expressive power is defined by the ontology language. While our work applies to a more general setting (see Section 3), below, we illustrate our discussion on the DL-Lite$_{\mathbb{Q}}$ description logic [13], which is the first order logic foundation of the W3C’s OWL2 QL standard for managing semantic-rich Web data. For what concerns expressive power, DL-Lite$_{\mathbb{Q}}$ is a significant extension of the subset of RDF (comprising RDF Schema) which can be translated into description logics, a.k.a. the DL fragment of RDFS; DL-Lite$_{\mathbb{Q}}$ is also a fragment of Datalog$^\pm$ [11].

Given a role $R$, its inverse, denoted $R^\text{−1}$, is the set: $\{(b, a) \mid R(a, b) \in A\}$. We denote $N^R_Z$ the set of roles made of all role names, together with their inverses: $N^R_Z = NR \cup \{r^\text{−1} \mid r \in NR\}$. For instance, supervisedBy and supervisedBy$^\text{−1}$, whose meaning is supervises, are in $N^R_Z$. A DL-Lite$_{\mathbb{Q}}$ TBox constraint is either:

(i) a concept inclusion of the form $C_1 \sqsubseteq C_2$ or $C_1 \sqsubseteq \neg C_2$, where each of $C_1, C_2$ is either a concept from $NC$, or $3R$ for some $R \in NR$, and $\neg C_2$ is the complement of $C_2$. Here, $\exists R$ denotes the set of constants occurring first in the position in role $R$ (i.e., the projection on the first attribute of $R$). For instance, $\exists_{\text{supervisedBy}}$ is the set of those supervised by somebody, while $\exists_{\text{supervisedBy}}^\text{−1}$ is the set of all supervisors (i.e., the projection on the first attribute of $\exists_{\text{supervisedBy}}$), hence on the second of $\exists_{\text{supervisedBy}}$;

(ii) a role inclusion of the form $R_1 \subseteq R_2$ or $R_1 \subseteq \neg R_2$, with $R_1, R_2 \in N^R_Z$.

Observe that the left-hand side of the constraints are negation-free; in DL-Lite$_{\mathbb{Q}}$, negation can only appear in the right-hand side of a constraint. Constraints featuring negation allow expressing a particular form of integrity constraints: disjointness or exclusion constraints. The next example illustrates DL-Lite$_{\mathbb{Q}}$ KBs.

**Example 1 (DL-Lite$_{\mathbb{Q}}$ KB).** Consider the DL-Lite$_{\mathbb{Q}}$ TBox $T$ in Table 2 expressing constraints on the Researcher and PhDStudent concepts, and the worksWith and supervisedBy roles. It states that PhD students are researchers (T1), researchers work with researchers (T2), working with someone is a symmetric relation (T4), being supervised by someone implies working with her/him.
Example 2 (DL-Lite\textsubscript{R} entailment). The KB $\mathcal{K} = \langle \mathcal{T}, \mathcal{A} \rangle$ from Example\textsubscript{1} entails many constraints and assertions. For instance:

- $\mathcal{K} \models \neg \text{supervisedBy} \sqsubseteq \neg \text{supervisedBy}$, i.e., the two attributes of supervisedBy are disjoint, due to (T6)+(T7):
- $\mathcal{K} \models \text{worksWith}(\text{Francois}, \text{Joana})$, i.e., Fran\-çois works with Joana, due to (T4)+ (A1):
- $\mathcal{K} \models \text{PhDStudent}(\text{Damian})$, i.e., Damian is a PhD student, due to (A2)+(T6):
- $\mathcal{K} \models \text{worksWith}(\text{Francois}, \text{Damian})$, i.e., Fran\-çois works with Damian, due to (A3)+(T7)+(T4).

Finally remark that $\mathcal{A}$ is $\mathcal{T}$-consistent, i.e., there is no violation of its only constraint using negation (T7), since the KB $\mathcal{K}$ does not entail that some PhD student supervises another.

2.2 Queries

A FOL query is of the form $q(x) \leftarrow \phi(x)$ where $\phi(x)$ is a FOL formula whose free variables are $x$; the query name is $q$, its head is $\phi(x)$, while its body is $\phi(x)$. Without loss of generality, in the sequel, we consider only connected queries, i.e., those which do not feature cartesian products. The answer set of a query $q$ against a knowledge base $\mathcal{K}$ is:

\[ \text{ans}(q, \mathcal{K}) = \{ t \in (N_{t})^{k} \mid \mathcal{K} \models \phi(t) \}. \]

where $\mathcal{K} \models \phi(t)$ means that every model of $\mathcal{K}$ is a model of $\phi(t)$. If $q$ is Boolean, $\text{ans}(q, \mathcal{K}) = \{ \} \cup \{ \}$ encodes true, with $\{ \}$ the empty tuple, while $\text{ans}(q, \mathcal{K}) = \{ \}$ encodes false. In keeping with the literature on query answering under ontological constraints, our queries have set semantics, i.e., a tuple either belongs to the answer or does not, but it cannot appear several times in the answer.

Example 3 (Query answering). Consider the FOL query $q$ asking for the PhD students with whom someone works:

\[ q(x) \leftarrow \exists y \text{PhDStudent}(x) \land \text{worksWith}(y, x). \]

Given the KB $\mathcal{K}$ of Example\textsubscript{2} the answer set of this query is $\{\text{Damian}\}$, since $\mathcal{K} \models \text{PhDStudent}(\text{Damian})$ and $\mathcal{K} \models \text{worksWith}(\text{Francois}, \text{Damian})$ hold. Observe that evaluating $q$ against $\mathcal{K}$’s ABox only yields no answer.

To simplify the reading, in what follows, we omit the quantifiers of existential variables, and simply write the above query as $q(x) \leftarrow \text{PhDStudent}(x) \land \text{worksWith}(y, x)$.

### Table 4: FOL query dialects.

<table>
<thead>
<tr>
<th>Query dialect</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CQ</td>
<td>$q(x) \leftarrow a_{1} \land \cdots \land a_{n}$</td>
</tr>
<tr>
<td>SCQ</td>
<td>$q(x) \leftarrow (a_{1}^{1} \lor \cdots \lor a_{1}^{k_{1}}) \land \cdots \land (a_{n}^{1} \lor \cdots \lor a_{n}^{k_{n}})$</td>
</tr>
<tr>
<td>UCQ</td>
<td>$q(x) \leftarrow CQ_{1}(x) \lor \cdots \lor CQ_{n}(x)$</td>
</tr>
<tr>
<td>USCQ</td>
<td>$q(x) \leftarrow USCQ_{1}(x) \lor \cdots \lor USCQ_{n}(x)$</td>
</tr>
<tr>
<td>JUCQ</td>
<td>$q(x) \leftarrow UJCQ_{1}(x_{1}) \land \cdots \land UJCQ_{n}(x_{n})$</td>
</tr>
<tr>
<td>JUSCQ</td>
<td>$q(x) \leftarrow JUSCQ_{1}(x_{1}) \land \cdots \land JUSCQ_{n}(x_{n})$</td>
</tr>
</tbody>
</table>
\[ q^1(x) \leftarrow \text{PhDStudent}(x) \land \text{worksWith}(y, x) \]
\[ q^2(x) \leftarrow \text{PhDStudent}(x) \land \text{worksWith}(x, y) \]
\[ q^3(x) \leftarrow \text{PhDStudent}(x) \land \text{supervisedBy}(y, x) \]
\[ q^4(x) \leftarrow \text{PhDStudent}(x) \land \text{supervisedBy}(y, x) \]
\[ q^5(x) \leftarrow \text{supervisedBy}(x, z) \land \text{worksWith}(y, x) \]
\[ q^6(x) \leftarrow \text{supervisedBy}(x, z) \land \text{worksWith}(x, y) \]
\[ q^7(x) \leftarrow \text{supervisedBy}(x, z) \land \text{supervisedBy}(y, x) \]
\[ q^8(x) \leftarrow \text{supervisedBy}(x, z) \land \text{supervisedBy}(y, x) \]
\[ q^9(x) \leftarrow \text{supervisedBy}(x, z) \land \text{supervisedBy}(y, x) \]
\[ q^{10}(x) \leftarrow \text{supervisedBy}(x, y) \]

**Table 5: Union terms in CQ-to-UCQ reformulation (Example 4).**

**Notations.** Unless otherwise specified, we systematically use \( q \) to refer to a CQ query, \( a_1, \ldots, a_n \) to designate the atoms in the body of \( q \), \( T \) to designate a DL-Lite\( _T \) TBox, and \( A \) for an ABox.

**FOL-reducibility of data management.** In a setting where query answering is FOL-reducible, there exists a FOL query \( q^{\text{FOL}} \) (computable from \( q \) and \( T \)) such that:

\[ \text{ans}(q, (T, A)) = \text{ans}(q^{\text{FOL}}, (\emptyset, A)) \]

for any \( T \)-consistent ABox \( A \). Thus, query answering reduces to: a first reasoning step to produce the FOL query from \( q \) and \( T \) (this is also known as reformulating the query using the constraints), and a second step which evaluates the reformulated query \( q^{\text{FOL}} \) in the standard fashion, only on the ABox (i.e., disregarding the TBox constraints). This can be done for instance by translating it into SQL and delegating the evaluation to an RDBMS. From a knowledge base perspective, this allows to take advantage of highly optimized data stores and query evaluation engines to answer queries. From the database perspective, this two-step approach enhances the power of RDBMSs, as it allows to compute answers based only on data stored in the ABox (i.e., the database), but also taking into account the deductive constraints and all their consequences (entailed facts and constraints).

As DL-Lite\( _R \), query answering is FOL reducible [13], the literature provides techniques for computing FOL reformulations of a CQ in settings related to DL-Lite\( _R \). These techniques produce (i) a UCQ w.r.t. a DL-Lite\( _R \) TBox, e.g., [13] [14] [30] [43] or extensions thereof using existential rules [20] or Datalog [35] [18], (ii) a USCQ [13] w.r.t. a set of existential rules generalizing a DL-Lite\( _R \) TBox, and (ii) a set of alternative equivalent JUCQs [19] w.r.t. an RDF database [17], whose RDF Schema constraints are the following four, out of the twenty-two, DL-Lite\( _R \) ones: (1) \( A \subseteq A' \), (4) \( \exists R \subseteq A \), (5) \( \exists R \subseteq A \) and (11) \( R \subseteq R \).

**CQ-to-UCQ reformulation for DL-Lite\( _R \).** We present the pioneering CQ-to-UCQ technique on which we rely to establish our results. These results extend to any other FOL reformulation techniques for DL-Lite\( _R \), e.g., optimized CQ-to-UCQ or CQ-to-USCQ reformulation techniques, since they produce equivalent FOL queries.

The technique of [13] relies on two operations: specializing a query atom into another by applying a negation-free constraint (recall Table 3 in the backward direction, and specializing two atoms into their most general unifier (mgu, in short). These operations are exhaustively applied to the input CQ; each operation generates a new CQ contained in the input CQ w.r.t. the TBox, because the new CQ was obtained by specializing one or two atoms of the previous CQ. The same process is then applied on the new CQs, and so on recursively until the set of generated CQs reaches a fixpoint. The finite union of the input CQ and of the generated ones forms the UCQ reformulation of the input CQ w.r.t. the TBox.

**Example 4 (CQ-to-UCQ reformulation).** Consider the query \( q(x) \leftarrow \text{PhDStudent}(x) \land \text{worksWith}(y, x) \) and KB \( K \) of the preceding examples. The UCQ reformulation of \( q \) is:

\[ q^{\text{UCQ}}(x) \leftarrow \bigvee_{i=1}^{10} q^i(x) \]

where \( q^1 \sim q^{10} \) appear in Table 3. In the table, \( q^i(x) \) has exactly the body of \( q \). \( q^i(x) \) is obtained from \( q \) by applying the constraint \((T4): \text{worksWith} \subseteq \text{worksWith}^+\), which is of the form (10) listed in Table 3. \((T4)\) is applied backward, in the following sense: the query asks for \( \text{worksWith}(x, y) \), and \((T4)\) tells us that one of the possible reasons why this may hold, is if \( \text{worksWith}(x, y) \) holds. Thus, \( q^i \) is contained within \( q \), in the sense that if \( q^i \) holds, \( q \) is also sure to hold, but the opposite is not true: intuitively, \( "q^i \) may hold for other reasons (thanks to other specializations of its atoms)" - and it is exactly the set of such other specializations which the technique explores.

Similarly, \( q^3 \) is obtained from \( q^1 \) by applying the constraint \((T5)\) backward on the atom \( \text{worksWith}(y, x) \), and \( q^1 \) from \( q^3 \) by applying \((T5)\) on \( \text{worksWith}(x, y) \). To obtain \( q^3 \) to \( q^3 \), we apply \((T6)\) backward on the atom \( \text{PhDStudent}(x) \) in \( q^1 \) to \( q^9 \). Finally, \( q^9 \) is obtained from \( q^3 \) through the mgu of its two atoms, namely \( \text{supervisedBy}(x, z) \land \text{supervisedBy}(y, x) \): \( q^{10} \) is similarly obtained from \( q^9 \).

**2.3 Evaluating reformulated subqueries can be (very) hard**

It is worth noting that the (naïve) exhaustive application of specialization steps leads, in general, to highly redundant reformulations w.r.t. the containment of their disjuncts. For instance, minimizing \( q^{\text{UCQ}} \) in the above example by eliminating disjuncts contained in another leads to:

\[ q^{\text{UCQ}}(x) \leftarrow \bigvee_{i=1}^{4} q^i(x) \lor q^{10}(x) \]

where the disjuncts appear in Table 3 they are all contained in \( q^{10} \). Minimal UCQ reformulations can be obviously processed more efficiently. However, they still repeat some computations, e.g., in the above example, \( \text{PhDStudent} \) is read three times, \( \text{worksWith} \) twice etc; in general, subqueries appearing in different union terms are repeatedly evaluated.

Common subexpression elimination (CSE) techniques aim at identifying repeated subexpressions in queries or plans, and reformulating them so that the expression is evaluated only once and its results are shared to increase performance; CSE is often used in a Multi-Query Optimization context (MQO). However, MQO is poorly supported in today’s main RDBMS engines[1]. As we will see, our approach, which starts with the TBox and data statistics, and ends by hand-on over a chosen reformulation to the RDBMS, never requires work to detect common (repeated) sub-expressions.

Another source of difficulty is the sheer size of reformulated queries; we exhibit some whose size (i.e., length of the SQL formulation) is above 2,000,000 characters. For instance, the minimal UCQ corresponding to query \( Q_{10} \) in our experiments (Section 6) is a union of 145 CQs, and runs in 5665 ms on DB2 and a database of 100 million facts. In contrast, the SQL translation of the best FOL reformulation identified by our approach reduces this to 156 ms (36 times faster), just by giving the engine a different (yet equivalent) SQLized FOL reformulation.

From an optimization viewpoint, the problem we are facing can be seen as follows. We aim at answering queries through RDBMSs in the presence of constraints, for FOL-reducible settings.

The standard UCQ reformulation (and other cost-ignorant ones) perform quite badly. The question is, then: is there an equivalent reformulation which would be evaluated more efficiently?

[1] We checked this on Postgres, DB2, and MySQL plans; according to Paul Larson (among the authors of [36]), no major RDBMS engine as of April 2016 has a comprehensive MQO approach.
To answer this, one is faced with a set of FOL (or, alternatively, SQL) reformulations whose size is potentially very high: exponential in the query size for non-redundant queries, larger yet if one considers, for instance, queries featuring semi-joins [7]; each query therein may be (very) large, have many unions etc. From these, one would need to find the one(s) best optimized and executed by the RDBMS; their very high number makes this utterly impractical.

The following sections present our alternative approach.

3. OPTIMIZATION FRAMEWORK

The performance of evaluating (the SQL translation of) a given FOL reformulation of a query through an RDBMS depends on several factors: (i) data properties (size, cardinalities, value distributions etc); (ii) the storage model, i.e., the concrete relations storing the ABox, possible indexes etc; (iii) the optimizer’s algorithm. Among these, (i) is completely determined by the dataset (the given ABox). On the storage model (ii), for generality, we make no assumption, other than requiring that FOL query reformulations can be translated into SQL on the underlying store. (We study several such concrete models experimentally, in Section 6). For what concerns optimizers (iii), we note that off-the-shelf they perform very poorly on previously proposed FOL query reformulations, yet we would like to exploit their strengths when possible.

Approach: cover-based query answering. We identify and exploit a novel space of alternative FOL reformulations of the given input CQ. We estimate the cost of evaluating each such reformulation through the RDBMS using standard database cost formulas, and hand to the RDBMS one with the best estimation.

More specifically, a query cover defines a way to split the query into subqueries, that may overlap, called fragment queries, such that substituting each subquery with its FOL reformulation (obtained from any state-of-the-art technique) and joining the corresponding reformulation (reformulated) subqueries, may yield a FOL reformulation of the original query (recall also Figure [1]).

Definition 1 (CQ cover). A cover of a query q, whose atoms are \{a_1, \ldots, a_n\}, is a set \(C = \{f_1, \ldots, f_m\}\) of non-empty subsets of atoms of q, called fragments, such that (i) \(\bigcup_{i=1}^{m} f_i = \{a_1, \ldots, a_n\}\), (ii) no fragment is included into another, and (iii) the atoms of each fragment are connected through joins (common variables).

Example 5 (CQ cover). Consider the query

\[
q(x, y) \leftarrow \text{teachesTo}(v, x) \land \text{teachesTo}(v, y) \land \text{supervisedBy}(x, w) \land \text{supervisedBy}(y, w)
\]

C, below, is a query cover for q:

\[
C = \{\{\text{teachesTo}(v, x) \land \text{supervisedBy}(x, w)\}, \{\text{teachesTo}(v, y) \land \text{supervisedBy}(y, w)\}\}
\]

Definition 2 (Fragment queries of a CQ). Let \(C = \{f_1, \ldots, f_m\}\) be a cover of q. A fragment query \(q_{f_i, \ldots, f_m}\) of q w.r.t. C is the subquery whose body consists of the atoms in \(f_i\) and whose free variables are the free variables x of q appearing in the atoms of \(f_i\), plus the existential variables in \(f_i\) that are shared with another fragment \(f_{j, \ldots, f_m}\), i.e., on which the two fragments join.

Example 6 (Fragment queries of a CQ). The fragment queries of the query \(q(x, y)\) w.r.t. the cover C (Example 5) are:

\[
q_{f_1}(x, v, w) \leftarrow \text{teachesTo}(v, x) \land \text{supervisedBy}(x, w)
\]

\[
q_{f_2}(y, v, w) \leftarrow \text{teachesTo}(v, y) \land \text{supervisedBy}(y, w)
\]

As we shall see in the next Section, not every cover of a query leads to a FOL reformulation. Specifically, we define:

Definition 3 (Cover-based reformulation). Let \(C = \{f_1, \ldots, f_m\}\) be a cover of q, and \(q^{\text{FOL}}(\bar{x}) \leftarrow \bigwedge_{i=1}^{m} q_{f_i}^{\text{FOL}}\), a FOL query, where \(q_{f_i}^{\text{FOL}}\), for 1 \(\leq i \leq m\), is a FOL reformulation w.r.t. \(T\) of the fragment query \(q_{f_i}\), of q.

\(q^{\text{FOL}}\) is a cover-based reformulation of q w.r.t. \(T\) and C if it is a FOL reformulation of q w.r.t. \(T\).

To exemplify cover-based FOL reformulations, one needs to choose a specific KB dialect, among all those enjoying FOL reducibility; we present examples in the next Section, when instantiating our framework to the DL-Lite\(_c\) setting.

For now, it helps to see how we derive the SQL query corresponding to the cover-based reformulation. Each reformulated fragment query \(q_{f_i}^{\text{FOL}}\) is translated into an SQL query \(q_{f_i}\); then, the overall query is of the form:

\[
\text{SELECT DISTINCT } \bar{y}_{f_1, \ldots, f_m} \text{ FROM } q_{f_1} \cap \ldots \cap q_{f_m}, \ldots, q_{f_1} \cap \ldots \cap q_{f_m}
\]

where \(\text{cond}(1, 2, \ldots, n)\) is the conjunction of the join predicates between all the subqueries. This leads to all the \(\text{WITH}\)-introduced subqueries being evaluated and materialized into intermediary table\(\bar{y}\) while the one with the largest number of results is run in pipeline fashion. The way in which each subquery is evaluated, then their results are joined, left to the DBMS to determine. The SELECT DISTINCT ensures set semantics for the query answers.

Problem statement. We assume given a query cost estimation function \(\epsilon\) which, for any FOL query q, returns the cost of evaluating it through an RDBMS storing the ABox. Thus, \(\epsilon\) reflects the operations (data access, joins, unions etc) applied on the ABox to compute the answers of a q\textsuperscript{FOL} reformulation. The cost estimation \(\epsilon\) also accounts for the effort needed to join the reformulated fragment query answers, in the most efficient way.

Problem 1 (Optimization problem). Given a CQ q and a KB \(K\), the cost-driven cover-based query answering problem consists of finding a cover-based reformulation of q based on \(K\) with lowest (estimated) evaluation cost.

A cost estimation function is provided by most RDBMSs storing the ABox for instance through the SQL explain directive. One can also estimate costs outside the engine using well-known textbook formulas, as in e.g., [10]. We use both options in our experiments.

4. COVER-BASED QUERY ANSWERING IN DL-Lite\(_c\)

We now instantiate our cover-based query answering technique to the popular setting of DL-Lite\(_c\). As already mentioned in Section 2, we use the simple CQ-to-USQ reformulation technique of [13] for establishing our results, and in our examples. However, our approach applies to any other FOL reformulation techniques for DL-Lite\(_c\), e.g., optimized CQ-to-USQ or CQ-to-UCQ reformulation techniques, since these produce equivalent (though possibly syntactically different) FOL queries.

Example 7 (Running example). Let \(K\) be the KB with TBox \(T = \{\text{Graduate} \sqsubseteq \exists \text{supervisedBy}. \text{supervisedBy} \sqsubseteq \text{worksWith}\}\) and ABox \(A = \{\text{PhDStudent}(\text{Damian}), \text{Graduate}(\text{Damian})\}\).

Consider the query \(q(x) \leftarrow \text{PhDStudent}(x) \land \text{worksWith}(x, y) \land \text{supervisedBy}(y, z)\), whose answer against \(K\) is \(\{\text{Damian}\}\).

\(^3\)For performance, these SQL subqueries use DISTINCT to reduce the size of the intermediate materialized results.
The UCQ reformulation of \( q \) is \( q_{\text{UCQ}}(x) \) with:

\[
q^1(x) \leftarrow \text{PhDStudent}(x) \land \text{worksWith}(x, y) \\
\land \text{supervisedBy}(y, z)
\]

\[
q^2(x) \leftarrow \text{PhDStudent}(x) \land \text{supervisedBy}(x, y) \\
\land \text{supervisedBy}(y, z)
\]

\[
q^3(x) \leftarrow \text{PhDStudent}(x) \land \text{supervisedBy}(y, z) \\
\land \text{supervisedBy}(x, y)
\]

\[
q^4(x) \leftarrow \text{PhDStudent}(x) \land \text{Graduate}(x)
\]

Above, \( q^1 \) has the body of \( q \); \( q^2 \) is obtained from \( q^1 \) by specializing the atom \text{worksWith}(x, y) through a backward application of \text{supervisedBy} \subseteq \text{worksWith}. \( q^3 \) (highlighted in blue) results from \( q^2 \) by replacing \text{supervisedBy}(x, y) and \text{supervisedBy}(y, z) with their most general uniform. \( q^4 \) is obtained from \( q^3 \), by specializing \text{supervisedBy}(x, y) through the backward application of \text{Graduate} \subseteq \text{supervisedBy}; we also show \( q^4 \) in blue to highlight its connection with \( q^3 \).

Now let \( C_1 = \{ \text{PhDStudent}(x), \text{worksWith}(x, y) \} \), \{\text{supervisedBy}(y, z)\} be a cover of \( q \). From Definition 2, the corresponding fragment queries are:

\[
q_1(x, y) \leftarrow \text{PhDStudent}(x) \land \text{worksWith}(x, y) \\
q_2(y) \leftarrow \text{supervisedBy}(y, z)
\]

The reformulation of \( q_1 \) using \( T \) is \( q_{\text{UCQ}}^1(x, y) \leftarrow \bigvee_{i=1}^4 q_i(x, y) \), where

\[
q^1_1(x, y) \leftarrow \text{PhDStudent}(x) \land \text{worksWith}(x, y) \\
q^2_1(x, y) \leftarrow \text{PhDStudent}(x) \land \text{supervisedBy}(x, y)
\]

\( q^2 \) is obtained from \( q^1_1 \) by the backward application of the constraint \text{supervisedBy} \subseteq \text{worksWith}.

The reformulation of \( q_2 \) using \( T \) is simply:

\[
q_{\text{UCQ}}^2(y) \leftarrow \text{supervisedBy}(y, z)
\]

By Definition 3, the reformulation of \( q \) using \( C_1 \) is the conjunct \( q_{\text{UCQ}}(x) \leftarrow q_{\text{UCQ}}^1(x, y) \land q_{\text{UCQ}}^2(y) \), which is clearly equivalent to the following UCQ obtained by distributing \( \land \) over \( \lor \):

\[
q_{\text{UCQ}}^1(x) \leftarrow (q^1(x, y) \land q_{\text{UCQ}}^2(y)) \lor (q^2_1(x, y) \land q_{\text{UCQ}}^2(y))
\]

where the first and second disjuncts correspond to the CQs:

\[
q^1_2(x) \leftarrow \text{PhDStudent}(x) \land \text{worksWith}(x, y) \\
\land \text{supervisedBy}(y, z)
\]

\[
q^2_2(x) \leftarrow \text{PhDStudent}(x) \land \text{supervisedBy}(x, y) \\
\land \text{supervisedBy}(y, z)
\]

Above, \( q^2_1(x) \) and \( q^2_2(x) \) are exactly \( q^1 \) and \( q^2 \) from the UCQ reformulation of \( q \) however, \( q^3 \) and \( q^4 \) are missing from \( q_{\text{UCQ}}^1(x) \). Since \( q^1 \) derives from \( q \), the absence of both can be traced to the absence of \( q^1 \). The reason \( C_1 \) does not lead to \( q^3 \) is that \text{supervisedBy}(x, y) \land \text{supervisedBy}(y, z) \) is not obtained while reformulating \( q^1_1(x, y) \), thus the unification of these two atoms (which could have lead to \( q^2_1 \)) is missed. In the CQ-to-UCQ reformulation of \( q \), \text{supervisedBy}(x, y) \land \text{supervisedBy}(y, z) \) appears in \( q^2 \) because \text{worksWith}(x, y) \land \text{supervisedBy}(y, z) \) appears in \( q^1 \). However, \( C_1 \) separates the \text{worksWith} and \text{supervisedBy} atoms in different fragments. Reformulating them independently misses exactly the opportunity to produce \( q^3 \) and \( q^4 \).

Due to these absent subqueries, \( q_{\text{UCQ}}^1 \) is not a FOL reformulation of \( q \) w.r.t. \( T \), i.e., it fails to compute \( q \)'s answer: \( \text{ans}(q_{\text{UCQ}}^1, (\emptyset, \mathcal{A})) = \emptyset \) while the answer of \( q \) against \( \mathcal{K} \) is \{Damian\}.

1Here, the \text{mgv} is \text{supervisedBy}(x, y) because \( x \) is the head variable; \( q^3 \) is equivalent to (and a minimal form of) \( q^2 \), but in general, \( q^3 \) is only guaranteed to be contained in (or equivalent to) \( q^2 \).

More generally, given an input \( CQ \) and a TBox, each pair of query atoms getting unifications during the CQ-to-UCQ reformulation of the whole query must not be separated by (must not be in different fragments of) a cover, in order for the corresponding cover-based reformulation to be a FOL reformulation. When this is the case, we say the cover is safe for query answering.

Thus, we are interested in a sufficient condition for a cover to be safe; intuitively, we must approximate (by some supersets) those sets of atoms which (directly or after some specializations) are pairwise unified by the CQ-to-UCQ algorithm, and ensure that each such atom set is in the same cover fragment.

Only atoms with the same predicate may unify. Thus, we identify for each predicate (i.e., concept or role name) occurring in a query, the set of all TBox predicates in which this predicate may turn through some sequence of atom specializations, i.e., backward constraint application and/or unification (the two operations applied by the technique of [13] which we consider here). This is captured by the classical notion of dependencies between predicates within knowledge bases, Datalog programs, etc. In DL-Lite\(_R\), this notion translates into the following recursive definition.

Definition 4 (Concept and role dependencies w.r.t. a TBox). Given a TBox \( T \), a concept or role name \( N \) depends w.r.t. \( T \) on the set of concept and role names denoted \( \text{dep}(N) \) and defined as the fixpoint of:

\[
\text{dep}^0(N) = \{ N \} \\
\text{dep}^{n+1}(N) = \text{dep}^n(N) \cup \{ \text{cr}(Y) \mid Y \subseteq X \in T \text{ and } \text{cr}(X) \in \text{dep}^{n-1}(N) \}
\]

where \( \text{cr}(Y) \) returns, for any input \( Y \) of the form \( Z, Z^- \) or \( \exists Z \) (for some concept or role \( Z \)), the concept or role name \( Z \) itself.

Example 8 (Predicate dependencies). In the TBox of Example 7

\[
\text{dep(PhDStudent)} = \{ \text{PhDStudent} \}
\]

\[
\text{dep(Gegraduate)} = \{ \text{Graduate} \}
\]

\[
\text{dep(worksWith)} = \{ \text{worksWith, supervisedBy, Graduate} \}
\]

\[
\text{dep(supervisedBy)} = \{ \text{supervisedBy, Graduate} \}
\]

Above, \text{worksWith} depends on \text{supervisedBy} because of the constraint \text{supervisedBy} \subseteq \text{worksWith}; similarly, \text{supervisedBy} depends on \text{Graduate} due to the constraint \text{Graduate} \subseteq \text{supervisedBy}, thus \text{worksWith} also depends on \text{Graduate}.

Definition 5 (Safe cover for query answering). A cover \( C \) of \( q \) is safe for query answering w.r.t. \( T \) (or safe in short) iff it is a partition of \( q \)'s atoms such that two atoms whose predicates depend on a common concept or role name w.r.t. \( T \) are in a same fragment.

Note that while Definition 5 requires covers to be partitions, we will relax this restriction in Section 5.2.

Theorem 1 (Cover-based query answering). Let \( C \) be a safe cover for \( q \) w.r.t. \( T \). The cover-based reformulation (Definition 5) of \( q \) based on \( C \), using any CQ-to-UCQ (resp. CQ-to-UCQ) reformulation technique, yields a cover-based reformulation \( \text{UCQ}^C \) of \( q \) w.r.t. \( T \).

Proof. The proof follows from that of correctness of the CQ-to-UCQ reformulation technique in [13] for query answering. It directly extends to the use of any CQ-to-UCQ or CQ-to-UCQ reformulation technique for DL-Lite\(_R\) as, for any CQ and TBox, the FOL queries they compute are equivalent to the query produced by the technique described in [13].

Soundness: for any \( T \)-consistent Abox \( \mathcal{A} \), \( \text{ans}(q_{\text{FOL}}, (\emptyset, \mathcal{A})) \subseteq \text{ans}(q, (T, \mathcal{A})) \) holds.
Let \( t \) be a tuple in \( \text{ans}(q^{\text{FOL}}, (\emptyset, \mathcal{A})) \). From Definition 3, \( q^{\text{FOL}} \) is \( q^{\text{FOL}}(x) \leftarrow \bigwedge_{i=1}^{m} q^{\text{FOL}}(x_i), \) thus \( t \) results from \( t_i \in \text{ans}(q^{\text{FOL}}, (\emptyset, \mathcal{A})) \), for \( 1 \leq i \leq m \). Therefore, for \( 1 \leq i \leq m \), \( t_i \in \text{ans}(q; (\mathcal{T}, \mathcal{A})) \) holds, because of the soundness of the CQ-to-UCQ reformulation technique. Hence, from Definition 3 \( t \in \text{ans}(q; (\mathcal{T}, \mathcal{A})) \) holds.

Completeness: for any \( \mathcal{T} \)-consistent Abox \( \mathcal{A} \), \( \text{ans}(q; (\mathcal{T}, \mathcal{A})) \subseteq \text{ans}(q^{\text{FOL}}, (\emptyset, \mathcal{A})) \).

Let \( t \) be a tuple in \( \text{ans}(q; (\mathcal{T}, \mathcal{A})) \). Let \( q^{\text{UCQ}} \) be its reformulation using the CQ-to-UCQ technique. From the completeness of this technique, \( t \in \text{ans}(q^{\text{UCQ}}, (\emptyset, \mathcal{A})) \). Let \( q^{\text{UCQ}} \) be \( \bigvee_{i=1}^{m} q^{\text{UCQ}}_i \), then necessarily for some \( t \in \text{ans}(q^{\text{UCQ}}, (\emptyset, \mathcal{A})) \) holds [13].

Let \( q^{\text{FOL}} \) be \( \bigwedge_{i=1}^{m} q^{\text{FOL}}_i \), \( \bigwedge_{i=1}^{m} \bigvee_{j=1}^{n} q^{\text{FOL}}_{i,j} \). Since Definition 5 makes the reformulation of each fragment independent from another w.r.t. the CQ-to-UCQ technique, for any \( q^{\text{UCQ}} \), \( q^{\text{FOL}} = \bigwedge_{i=1}^{m} q^{\text{FOL}}_i \). Hence, \( t \in \text{ans}(q^{\text{FOL}}, (\emptyset, \mathcal{A})) \).

If a CQ-to-UCQ reformulation algorithm is used on fragment queries, the cover-based reformulation will be a JUCQ; otherwise, a CQ-to-USCQ reformulation of the fragment queries lead to a JUSCQ reformulation.

Note that the trivial one-fragment cover (comprising all query atoms) is always safe; in this case, our query answering technique reduces to just one reformulation, the CQ-to-UCQ one identified by previous reformulation algorithms from the literature.

Example 9 (JUCQ reformulation with a safe cover). We now consider the safe cover \( C_2 = \{ \text{PhDStudent}(x) \}, \{ \text{worksWith}(x, y), \text{supervisedBy}(z, y) \} \). The cover-based reformulation based on \( C_2 \) the JUCQ query \( q^{\text{UCQ}} \) \( \leftarrow q^{\text{UCQ}}_1(x) \land q^{\text{UCQ}}_2(x) \), where:

\[
q^{\text{UCQ}}_1(x) \leftarrow \text{PhDStudent}(x) \\
q^{\text{UCQ}}_2(x) \leftarrow (\text{worksWith}(x, y) \land \text{supervisedBy}(z, y)) \\
\quad \lor (\text{supervisedBy}(x, y) \land \text{supervisedBy}(z, y)) \\
\quad \lor \text{Graduate}(x)
\]

Observe that \( \text{ans}(q^{\text{UCQ}}, (\emptyset, \mathcal{A})) = \{ \text{Damian} \} = \text{ans}(q; (\mathcal{T}, \mathcal{A})) \).

5. COVER-BASED QUERY OPTIMIZATION IN DL-Lite\(_R\)

We study now the query answering optimization problem of Section 3 for DL-Lite\(_R\). We analyze a first optimization space in Section 5.1 before extending our discussion to a larger space in Section 5.2. Finally, we describe our search algorithms in Section 5.3.

5.1 Safe covers optimization space

Below, we study the space of safe covers for a given query and TBox. We start by identifying a particularly interesting one:

Definition 6 (Root cover). We term root cover for a query \( q \) and TBox \( \mathcal{T} \) the cover \( C_{\text{root}} \) obtained as follows. Start with a cover \( C_1 \) where each atom is alone in a fragment. Then, for any pair of fragments \( f_1, f_2 \subseteq C_1 \) and atoms \( a_1 \in f_1, a_2 \in f_2 \) such that there exists a predicate on which those of \( a_1 \) and \( a_2 \) depend w.r.t. \( \mathcal{T} \), create a fragment \( f' = f_1 \cup f_2 \) and a new cover \( C_2 = (C_1 \setminus \{ f_1, f_2 \}) \cup \{ f' \} \). Repeat the above until the cover is stationary; this is the root cover, denoted \( C_{\text{root}} \).

It is easy to see that \( C_{\text{root}} \) does not depend on the order in which the fragments are considered (due to the inflationary method building it). Further, \( C_{\text{root}} \) is safe, given that it keeps in a single fragment any two atoms whose predicates may be unified.

The following important lemma characterizes the structure of \( C_{\text{root}} \) fragments:

Lemma 1 (\( C_{\text{root}} \) fragment structure). A fragment \( f \) in the root cover \( C_{\text{root}} \) is of one of the following two forms:

1. a singleton, i.e., \( f = \{ a_i \} \) for some query atom \( a_i \);
2. \( f = \{ a_{i1}, \ldots, a_{in} \} \), for \( n \geq 2 \), and for every atom \( a_{i1} \in f \), there exists one atom \( a_{i2} \in f \) and a predicate \( b_j \) in the TBox, such that both the predicates of \( a_{i1} \) and of \( a_{i2} \) depend on \( b_j \).

Proof. The lemma follows directly from the definition of \( C_{\text{root}} \).

Those atoms that do not share a dependency with any other atom appear in singleton fragments (case 1 above, as the construction of the root cover never groups them together). Atoms which share some dependencies (i.e., atoms whose predicates depend on one another) get unioned in fragments of the form 2 above.

Example 10 (Root cover). On the query and TBox from Example 7 the root cover is \( C_2 \) from Example 2 \( \text{worksWith}(x, y) \) and \( \text{supervisedBy}(z, y) \) are in the same \( C_2 \) fragment because \( \text{worksWith} \) depends on \( \text{supervisedBy} \) (cf. Example 8).

Proposition 1 states that \( C_{\text{root}} \) has the maximal number of fragments (equivalently, it has the smallest fragments) among all the safe covers for \( q \) and \( \mathcal{T} \); its proof is based on Lemma 1.

Proposition 1 (Minimality of \( C_{\text{root}} \) fragments). Let \( C_{\text{root}} \) be the root cover for \( q \) and \( \mathcal{T} \), and \( C \) be another safe cover. For any fragment \( f \subseteq C_{\text{root}} \), and atoms \( a_1, a_2 \in f \), there exists a fragment \( f' \subseteq C \) such that \( a_1, a_2 \in f' \), in other words: any pair of atoms together in \( C_{\text{root}} \) are also together in \( C \).

From Proposition 1 we obtain:

Theorem 2 (Safe cover space). Let \( C \) be a safe cover and \( f \) one of its fragments. Then, \( f \) is the union of some fragments from \( C_{\text{root}} \).

Proof. Suppose that \( f \) is not a union of some fragments from \( C_{\text{root}} \), and let us show a contradiction. In this case, \( f \) necessarily contains a strict, non-empty subset of a fragment of \( C_{\text{root}} \). It follows that there are two atoms whose predicates depend on a common concept or role name w.r.t. \( \mathcal{T} \), as they were together in the fragment of \( C_{\text{root}} \) that are not in a same fragment of \( C \). Therefore \( C \) is not a safe cover, a contradiction.

Safe cover lattice. Theorem 2 entails that the safe covers of a query \( q \) form a lattice, denoted \( L_q \), whose precedence relationship is denoted \( \preceq \), where \( C_1 \preceq C_2 \) iff each fragment of \( C_2 \) is a union of some fragments of \( C_1 \). The lattice has as lower bound the single-fragment cover, and as upper bound the root cover. For convenience, we also use \( L_q \) to denote the set of all safe covers.

The size of the safe cover lattice is bounded by the number of partitions of the query atoms, a.k.a. the Bell number \( B_n \), for a query of \( n \) atoms; the bound occurs when there is no dependency between the atom predicates.

5.2 Generalized covers optimization space

A dependency-rich TBox leads to few, large fragments in \( C_{\text{root}} \), thus to a relatively small number of alternative cover-based reformulations. In this section, we explore a notion of generalized covers, and propose a method for deriving FOL query reformulations from such covers. This enlarges our space of alternatives and thus potentially leads to a better cost-based choice of reformulation.

We call generalized fragment of a query \( q \) and denote \( f \mid g \) a pair of \( q \) atoms sets such that \( g \subseteq f \). A generalized cover is a set of generalized fragments \( C = \{ f_1\|g_1, \ldots, f_m\|g_m \} \) of a query \( q \).
such that $\cup_{1 \leq i \leq m} f_i$ is the set of atoms of the query, and no $f_i$ is included in $f_j$, for $1 \leq i \neq j \leq m$.

To a generalized fragment $f \mid g$ of a generalized cover $C$, we associate:

**Definition 7 (Generalized fragment query of a CQ).** The generalized fragment query $q_{f \mid g}$ of $q$ w.r.t. $C$ is the subquery whose body consists of the atoms in $f$, and whose free variables are the free variables of $q$ appearing in the atoms of $g$, plus the variables appearing in an atom of $q$ that are shared with some atom in $g$, for some other generalized fragment $f' \mid g'$ of $C$.

In a generalized fragment query, atoms from $f \setminus g$ only reduce (filter) the answers, without adding variables to the head. In particular, if $f = g$, $q_{f \mid g}$ coincides with the regular fragment query (Definition 2).

Given a generalized cover, the **generalized cover-based reformulation of a query** $q$ is the FOL query

$$q^g(x) \leftarrow \bigwedge_{i=1}^{m} q^{FOL}_{f_i \mid g_i}$$

if $q^g$ is a FOL reformulation.

If $f_i = g_i$ for all the fragments $f_i \mid g_i$, the generalized cover-based reformulation coincides with the regular cover-based one (Definition 2). As for simple cover-based reformulations, if fragments are reformulated into UCQs, the reformulated query is a JUCQ, whereas if they are reformulated into UCQs, the reformulated query is a JUSCQ.

The introduction of extra atoms in generalized fragments is reminiscent of the classical semijoin reducers [7], whereas one computes $R(x, y) \bowtie_y S(y, z)$ by

$$(R(x, y) \bowtie_y \pi_y(S(y, z))) \bowtie_y S(y, z)$$

where $\bowtie_y$ denotes the left semijoin, returning every tuple from the left-hand side input that joins with the right-hand input. The semijoin filters ("reduces") the $R$ relation to only those tuples having a match in $S$. If there are few distinct values of $y$ in $S$, $\pi_y(S(y, z))$ is small, thus the $\bowtie_y$ operator can be evaluated very efficiently. Further, if only few $R$ tuples survive the $\bowtie_y$ operator likely decreases with the size of its input.

While the benefits of semijoins are well-known, there are many ways to introduce them in a given query, increasing the space of alternative plans to be considered by an optimizer. While some heuristics have been proposed to explore only some carefully chosen semijoin plans [23], we noted that RDBMS optimizers do not explore semijoin options, in particular for the very large queries resulting from the FOL reformulations of CQs. Generalized fragments mitigate this problem by intelligently using semijoin reducers to fasten the evaluation of the FOL reformulation by the RDBMS.

**Generalized search space.** We now define the space $G_q$ of generalized covers for a given query $q$, based on the safe cover set $\mathcal{L}_q$. A generalized cover $C = \{f_1 \mid g_1, \ldots, f_m \mid g_m\}$ is part of $G_q$ iff:

- The cover $C_i = \{g_1, \ldots, g_m\}$ is safe, i.e., $C_i \in \mathcal{L}_q$;
- For each $1 \leq i \leq m$, the atoms in $f_i$ form a connected graph.

Note that an atom $a \in f$, for $f \mid g \in C$, has no impact on the head of the corresponding generalized fragment query; only the body of this query changes.

The size of $G_q$ obviously admits that of $\mathcal{L}_q$ as a lower bound. For a query $q$ of $n$ atoms, a upper bound is $B_n \times 2^{n-1}$, where $B_n$ is the $n$-th Bell number: for each safe cover $C'$ (of which there are at most $B_n$, see the previous section), each of the $n$ atoms may, in the worst case, be added or not to all the fragments to which it does not belong. In the worst case, there are $n-1$ such fragments.

The core result allowing us to benefit of the performance savings of generalized covers in order to efficiently answer queries is:

**Theorem 3 ($G_q$ cover-based query answering).** The reformulation of a query $q$ based on $\mathcal{T}$ and a generalized cover $C \in G_q$ is a FOL reformulation of $q$ w.r.t. $\mathcal{T}$.

**Proof.** The proof follows from that of Theorem 2. It relies on the fact that, given a safe cover $C = \{g_1, \ldots, g_m\}$ of $q$ and a generalized cover $C' = \{f_1 \mid g_1, \ldots, f_m \mid g_m\}$ of $q$, the queries $q'(x) \leftarrow \bigwedge_{i=1}^{m} q_{f_i \mid g_i}$, and $q'(x) \leftarrow \bigwedge_{i=1}^{m} q_{f_i \mid g_i}$, are equivalent, though each $g_i$ subsumes $f_i \mid g_i$. Indeed, $q'$ is obtained from $q$ by duplicating atoms already present in $q$, thus $q'$ only adds redundancy w.r.t. $q$; hence remains equivalent to it.

**Example 11 (General cover-based reformulation).** Recall the query and KB from Example 2. Let $f_0 = \{\text{PhDStudent}(x)\}$ and $f_1 = \{\text{worksWith}(x, y), \text{supervisedBy}(y, z)\}$ be the two fragments of the root cover $C_{\text{root}}$. Consider also the generalized cover $C_0 = \{f_1 \mid f_2 \mid f_0\}$, where $f_2 = \{\text{PhDStudent}(x), \text{worksWith}(y, x)\}$.

The generalized fragment query $q_{f_1 \mid f_0}$ of $q$ w.r.t. $C_0$ is the subquery $q_{f_1 \mid f_0}(x) \leftarrow \text{worksWith}(x, y) \land \text{supervisedBy}(y, z)$, where $y$ is not a free variable of $q_{f_1 \mid f_0}$ as it is neither a free variable of $q$ nor a variable in $f_0$, whereas $f_2 \mid f_0$ is the only other fragment in the cover $C_0$.

The generalized fragment query $q_{f_2 \mid f_0}$ of $q$ w.r.t. $C_0$ is the subquery $q_{f_2 \mid f_0}(x) \leftarrow \text{PhDStudent}(x) \land \text{worksWith}(y, x)$. Again, note that $y$ is not a (free) variable of $f_0$, and therefore it is not a free variable of $q_{f_2 \mid f_0}$.

Then, the generalized cover-based reformulation corresponding to $C_0$ is the FOL query:

$$q^g(x) \leftarrow q^{FOL}_{f_1 \mid f_0}(x) \land q^{FOL}_{f_2 \mid f_0}(x)$$

where:

$$q^{FOL}_{f_1 \mid f_0}(x) \leftarrow (\text{worksWith}(x, y) \land \text{supervisedBy}(y, z))$$

$\lor \text{supervisedBy}(y, x) \lor \text{Graduate}(x)$

$$q^{FOL}_{f_2 \mid f_0}(x) \leftarrow (\text{PhDStudent}(x) \land \text{worksWith}(y, x))$$

$\lor (\text{PhDStudent}(x) \land \text{supervisedBy}(y, x))$

$\lor (\text{PhDStudent}(x) \land \text{Graduate}(x))$

Applying supervisedBy $\sqsubseteq \text{worksWith}$ to $q_{f_1 \mid f_0}$ leads to:

$$(\text{worksWith}(x, y) \land \text{supervisedBy}(y, z))$$

$\lor (\text{supervisedBy}(y, x) \land \text{supervisedBy}(y, z))$$

$\lor (\text{supervisedBy}(y, x) \land \text{Graduate}(x))$

Then, applying Graduate $\sqsubseteq \exists\text{supervisedBy}$, we obtain the reformulation of $q_{f_1 \mid f_0}$ w.r.t. TBox $\mathcal{T}$, i.e., $q^{FOL}_{f_2 \mid f_0}$. Similarly, applying to $q_{f_2 \mid f_0}$ the constraint $\exists\text{supervisedBy}$ $\sqsubseteq \text{worksWith}$ and subsequently Graduate $\sqsubseteq \exists\text{supervisedBy}$ leads to $q^{FOL}_{f_2 \mid f_0}$.

Note that $\text{ans}(q^g, \{q, \mathcal{T}\}) = \{\text{Damian}\} = \text{ans}(q, \{\mathcal{T}\})$.

**5.3 Cost-based cover search algorithms**

Our first algorithm, EDL (Exhaustive Covers for DL), starts from $C_{\text{root}}$ and builds all $\mathcal{L}_q$ covers by unioning fragments, and all $G_q$ covers by adding atoms; the algorithm appears in [23].

The second one, GDL (Greedy Covers for DL) (Algorithm 1) works in a greedy fashion. It is based on exploring, from a given cover $C$, the set of possible next moves (lines 24 and 27); these are all the covers that may be created from $C$ by unioning two of its fragments or by enlarging one of its fragments, i.e., turning a fragment $f \mid g$ into $f \cup \{a\} \mid g$ for some query atom $a$ sharing a variable
with \( f \). The best one seen at a given point (w.r.t. the estimated evaluation cost) is kept as the selected next move in the \( \text{move} \) variable. At the end of this exploration step (line 7), the best move is applied, leading to the new best cover \( C \) from which the next exploration step starts. The exploration stops when no possible next move improves the cost of the currently selected best cover \( C \).

When unifying two fragments, \( \epsilon \) decreases if the resulting fragment is more selective than the two fragments it replaces. Therefore, the RDBMS may find a more efficient way to evaluate the query of this fragment, and/or its result may be smaller, making the evaluation of \( q^{\text{FOL}} \) based on the new cover \( C \) faster. When adding an atom to an extended fragment, \( \epsilon \) decreases if the conditions are met for the semijoin reducer to be effective (Section 5.2). In our context, many such opportunities exist, as our experiments show.

6. EXPERIMENTAL EVALUATION

We implemented our cover-based query answering approach in Java 8; the source code has about 10 000 lines, including the statistics and cost estimation (see below).

6.1 Experimental settings

First, we used PostgreSQL v9.3.2 to store the data and evaluate FOL query reformulations. We stored a unary table for each concept and a binary table for each role, and built all one- and two-attribute indexes, respectively, on those tables.

Second, we used the IBM DB2 Express-C 10.5. We chose it because (i) we found out in prior work [10] (and confirm below) that it evaluates large FOL reformulations better than Postgres, and (ii) it provides a relatively recent, smart storage layout for RDF graphs [9], intelligently bundling assertions into a small set of tables with potentially many attributes, so that the roles to which an individual participates are stored, to the extent possible, in the same tuple. This reduces the number of joins needed for query evaluation, and has been shown [9] to improve query performance. However, DB2 does not support reasoning, i.e., it only provides query evaluation. For DB2, we report results based on the concept and role tables (denoted simple layout) and on the RDF layout of [9].

In the simple layout, as customary in efficient Semantic Web data management systems, e.g., [28], facts are dictionary-encoded into integers, prior to storing them in the RDBMS. The TBox and predicates dependencies are stored in memory.

Hardware. The database servers ran on an 8-core Intel Xeon E5506 2.13 GHz machine with 16GB RAM, using Mandriva Linux r2010.0.

Datasets, queries, and reformulation engine. We used two LUBM9 benchmark KBs, comprising a DL-Lite\(_R\) TBox and two ABoxes of 15 million, respectively, 100 million facts, obtained using the EUDG data generator [23]. The TBox consists of 34 roles, 128 concepts and 212 constraints.

We devised a set of 13 CQs, reported in [8]. The queries have between 2 and 10 atoms, with an average of 5.77 atoms. Their UCQ reformulations are unions of 35 to 667 CQs, 290.2 on average. This parameter characterizing the query can be seen as a (rough) measure of the complexity of its reformulation.

We relied on the RAPID [14] CQ-to-UCQ reformulation tool to reformulate (simple or generalized) fragment queries (Definitions 2 and 4; any other CQ-to-UCQ or CQ-to-USCQ reformulation technique could have been used instead.

Cost estimation function. For the cost function estimation \( \epsilon \), we first used the RDBMS cost estimation for the SQL translation of each candidate FOL reformulation produced by our algorithms (\texttt{explain} in Postgres and \texttt{db22exppln} in DB2).

Further, for the simple layout, we implemented our own Java-based cost estimation, based on statistics on the stored data (cardinality and number of distinct values in each stored table attribute), and on the uniform distribution and independent distributions assumptions. Better RDF cardinality estimation techniques such as [27] may be used to improve the accuracy of our cost model.

Our cost model assumes joins run in linear time in the size of the input (e.g., hash joins when sufficient memory is available), and estimates data access costs by comparing all the applicable indexes. We calibrated the cost model for each of Postgres and DB2, by empirically determining the values of a few constant coefficients of the cost model formulas. The cost model is detailed in [6].

6.2 Search space and EDL running time

We first studied the number of covers in \( L_2 \) and \( G_\epsilon \) (recall Section 5). Our workload features some queries of 2 atoms, and the immediately larger ones have 6; the number of generalized covers is prohibitively high for 6 or more atoms. Thus, we derived from our first (six-atoms) query \( Q_1 \) a set of queries \( A_i \), \( 3 \leq i \leq 6 \), each of which is a star-join of \( i \) atoms on a common subject; in particular, \( A_6 \) is \( Q_1 \). The sizes of the resulting search spaces are reported in Table 6 for \( A_6 \) we stopped the search at 20 003 generalized covers (there were more). This demonstrates that exploring the full \( G_\epsilon \) space is in general not feasible. Thus, in the sequel, we do not use EDL for our tests, as it is impractical beyond (very) small queries. Table 6 also shows the number of covers explored by the greedy GDL; these grow very moderately with the query size.

Finally, for \( A_3-A_6 \), the running times of the best reformulation found by EDL and GDL (limited at 20 000 covers for \( A_6 \)) coincided. In general this is not guaranteed, but it is still an encouraging indicator of the good options found by GDL.

6.3 Evaluation time of reformulated queries

Figure 2 depicts the evaluation time, using Postgres with the simple layout, of four FOL reformulations:

1. the \( \text{UCQ} \) produced by the RAPID [14] reformulation engine;
2. the \( \text{JUCQ} \) reformulation based on \( C_{\text{not}} \);
3. the \( \text{JUCQ} \) reformulation corresponding to the best-performing (safe or generalized) cover, found by our algorithm GDL, using Postgres’ cost estimation (RDBMS);
4. the UCQ reformulation corresponding to the best-performing (safe or generalized) cover, found by our algorithm GDL, using our cost estimation (ext).

GDL running time is not reported in these graphs (see Section 6.4). We first analyze the top graph corresponding to LUBM\(^2\) 15M. It shows, first, that the UCQ reformulation is inefficient (one order of magnitude slower than the best reformulation found, e.g., for \(Q_5\) and \(Q_6\)). Second, the cover derived from \(C_{root}\) may also be very inefficient, in some cases (\(Q_6, Q_8, Q_{13}\)) much worse than the UCQ. These are both very large and complex queries; Figure 2 demonstrates that Postgres’ optimizer called directly on the fixed-form reformulation may performed quite poorly. The GDL-selected covers, in contrast, lead to the best-performing reformulations for all queries (often by an order of magnitude). Thus, our cost-based approach helps ask the RDBMS the optimization question it can best answer, among its equivalent formulations from the search space \(\mathcal{G}_q\). Striking exceptions are \(Q_8, Q_{10}\) which have both many atoms and complex reformulations, and \(Q_{11}\) which has 2 atoms but the maximum number (667) of reformulations. Here, the GDL reformulations selected using the RDFMS cost model perform very poorly, whereas the ones based on our own cost estimation are much faster. This may be because Postgres takes drastic shortcuts when estimating the cost of an extremely large query; in contrast, our cost estimation treats uniformly queries of all sizes. Recall that Postgres’ optimizer always has the last word in choosing how to evaluate the reformulation we select, using its own cost model. Thus, the difference can only be attributed to the cost estimation.

The bottom graph in Figure 2 corresponds to LUBM\(^2\) 100M; note the logarithmic y axis. Overall, the findings are the same: the UCQ and (especially in this case) the \(C_{root}\)-derived reformulation perform poorly, while those picked by GDL are faster than the standard UCQ by a factor of up to 6.6 (\(Q_2\)).

Table 6: Search spaces for queries \(A_3\) to \(A_6\).

<table>
<thead>
<tr>
<th>Query</th>
<th>(A_3)</th>
<th>(A_4)</th>
<th>(A_5)</th>
<th>(A_6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Q_9)</td>
<td>4</td>
<td>67</td>
<td>5674</td>
<td>&gt; 20000</td>
</tr>
<tr>
<td>(y_9) covers explored by GDL</td>
<td>2</td>
<td>5</td>
<td>11</td>
<td>18</td>
</tr>
<tr>
<td>(y_9) covers explored by GDL</td>
<td>12</td>
<td>27</td>
<td>59</td>
<td></td>
</tr>
</tbody>
</table>

Evaluation on DB2. The graph at the top of Figure 3 shows the evaluation time for DB2, on LUBM\(^2\) 15M, of seven reformulations: the same four which we ran on Postgres, to which we add, on the RDF layout [9]: the UCQ reformulation, the one based on \(C_{root}\), and the ones selected by GDL with the help of the RDFMS cost model. We did not code a cost estimation corresponding to this RDF-specific store, since (i) an accurate model of data access costs under such a complex layout (determined by running a linear programming solver etc.) seemed very hard to attain outside the server and (ii) DB2’s cost model performed similarly to (or better than) ours for all the GDL-selected covers, on the simple layout. Thus, replacing it with our own seemed unlikely to improve the performance. Note the logarithmic y axis of the graph.

First, note that five bars are missing (replaced by the vertical lines), one for \(Q_4\) and four for \(Q_{10}\). They all correspond to reformulations against the RDF layout. The server error was “The statement is too long or too complex. Current SQL statement size is 2,247,118” for the UCQ of \(Q_9\), and the same error (with similar query sizes) in the other cases. This shows that the cumulated impact of, first, the DB2RDF storage layout (which leads to 1F... THEN... ELSE and nesting in the SQL query corresponding to a simple CQ), and second, of ontology-based reformulation, yields queries too large for evaluation. For illustration, the SQL versions of \(Q_1\) before and after UCQ reformulation on DB2’s RDF store appear at [http://bit.ly/1TqeVMA](http://bit.ly/1TqeVMA). In cases where DB2 handled them, the reformulations corresponding to the UCQ, \(C_{root}\); and GDL on the RDF layout performed very poorly, up to 1 (UCQ) or even 4 \((C_{root})\) orders of magnitude worse than the best reformulations identified. Thus, our (somewhat unexpected) conclusion is that the RDF-specific layout, while interesting for CQ evaluation, is not the best alternative when evaluating queries issued from reformulation against an ontology.

Focusing only on the simple layout, we see that the cost-unaware UCQ and \(C_{root}\)-derived reformulations perform again poorly, while the GDL ones perform best and in many cases coincide. The two cost estimations behaved mostly the same, except that our estimation worked better for \(Q_4\) and worse for \(Q_9\). Overall, our chosen reformulations lead to performance gains of up to a factor of 9 w.r.t. the UCQ and/or \(C_{root}\) on the simple layout, for which we found DB2’s cost estimation quite reliable.

At the bottom of Figure 3 we show the evaluation times on LUBM\(^2\) 100M for the first eight among the ten reformulations shown in the top graph (we gave up GDL on the RDF layout, given our experience on the smaller dataset). The four execution errors (grey vertical lines) on the UCQ and \(C_{root}\) reformulations on the RDF layout are again due to overly large SQL queries. The first four alternatives are overall the worse, with \(C_{root}\) and at a lesser extent UCQ on the RDF layout performing very poorly. When focusing on the simple layout only, we notice that the cost-based reformulations improve over the simple UCQ performance by a factor of up to 36 (4.85 on average). There is an exception for \(Q_6\), where the UCQ was best; in this case, both DB2’s and our cost estimations were inaccurate, which we believe cannot be avoided in all cases. DB2’s estimation lead to significantly better reformulations than ours for the queries \(Q_2, Q_8, Q_9\) and \(Q_{12}\), while our cost model was clearly better for \(Q_{13}\). Overall, we found DB2’s cost estimation more accurate than our own (while the opposite holds...
for Postgres). By inspecting query plans, we confirmed that DB2 and Postgres do not apply any CSE across union terms. The better performance of DB2 is likely due to efficient runtime support for repeated scans [21].

In all experiments presented in this section, GDL ran between 1 ms (for 2-atom queries) to 207 ms (for the larger Q1); this includes the time to estimate costs using our model. Asking for RDBMSs’ cost estimations is more expensive, as we report in [8]: when the estimation is accessible through JDBC, the overhead may still be interesting given the performance savings.

Finally, always (when using our cost model) and about half of the time (with the RDBMS cost model), GDL picked a generalized cover. This confirms the interest of searching in the $G_q$ space.

6.4 Time-limited GDL

We have measured the running time of algorithm GDL, and found that in all cases, most of its running time is spent estimating reformulation costs: GDL running time other than cost estimation is at most 24 ms; the time spent estimating costs with our Java-based model is up to 100 ms; cost estimation through Postgres (accessed via JDBC) takes up to $10^6$ ms, and cost estimation through DB2 is up to $10^7$ ms. Cost estimation times grow with the size of the query (and is 1 ms for all algorithms for the smallest queries of 2 atoms). Clearly, the overhead of cost estimations through Postgres and DB2 (through JDBC calls, respectively, a system call to an executable DB2 utility) can be prohibitive.

Time-limited GDL. Therefore, we investigated a time-limited version of GDL, which we stopped after 20 ms. We compared the running time of the cover found by GDL after only 20 ms, with that of the cover found by GDL allowed to run to completion. We found [8] that the running times are quite close, demonstrating that interesting covers are quickly found. Thus, we find time-limited GDL performs well in practice, for a modest overhead.

6.5 Experiment conclusions

Our experiments show that plain UCQ reformulation is evaluated poorly by both Postgres and DB2, even more so (or even fails) on DB2’s RDF-specific data layout. On the simple layout, the fixed cover-based reformulation corresponding to the root cover $C_{\text{root}}$ also performs very poorly. In contrast, GDL-selected reformulation improve over the UCQ in all 13 queries $\times$ 2 systems $\times$ 2 datasets but one, and they do so by up to a factor of 36. Our cost estimation helped w.r.t. Postgres’ explain, but when using DB2, we find db2explain’s estimation more accurate overall.

The generalized cover space has prohibitive size, thus EDL is impractical. In contrast, our greedy GDL is efficient when used with a low-overhead cost estimation (such as the one we implemented), and effective in optimizing reformulated queries. GDL attains most of its cost reductions early on during the search, making it a robust tool for improving reformulated query answering performance.

7. RELATED WORK AND CONCLUSION

We proposed a novel framework for any OBDA setting enjoying FOL reducibility of query answering, for which we studied a space of alternative FOL reformulations to evaluate through an RDBMS. We applied this framework to the DL-Lite$\varepsilon$ description logic, and experimentally demonstrated its performance benefits.

Our approach departs from the literature focused on a single FOL query reformulation, where optimization mainly reduces to producing fast a UCQ reformulation as minimized as possible. [14] [15] [14] [20] [29] [18] consider DL-Lite$\varepsilon$, existential rules and Datalog$\varepsilon$; [33] studies CQ-to-USCQ reformulation for existential rules encompassing DL-Lite$\varepsilon$; USCQ reformulations are shown to perform overall better than UCQ ones in an RDBMS. We build on these works to devise CQ-to-JUCQ and CQ-to-JUSCQ reformulation techniques, and used cost estimations to speed up reformulated query evaluation. Our generalized covers can be seen as adapting semijoin-based reducers to the query answering setting. [31] proposes a cost-unaware CQ-to-Datalog reformulation technique: it produces a non-recursive Datalog program, which amounts to a JUCQ.

One contribution of this work is an optimization framework (Section 5) for any formalism for which query answering is FOL-reducible, e.g., some Description Logics, Datalog$\varepsilon$ and Existential
Rules fragments. Our previous work is a particular case of this framework for the RDFS ontology language, which corresponds only to the constraints 1, 4, 5 and 11 from Table 3 while the DL-LiteR language we use (foundational for W3C’s standard for very large Semantic Web data management OWL2 QL) comprises 22 such constraints. When reformulating under this rich language, some covers are unsafe (recall Example 7), while in any cover leads to a correct query reformulation for the 4 constraints considered there. Thus, the other contributions of our work are: to identify and characterize safe covers, guaranteed to lead to reformulations, and a carefully chosen extra space of generalized covers which lead to equivalent FOL reformulations and often improve query performance. Our EDL and GDL optimization algorithms (Section 5.3) respectively explore exhaustively and greedily this DL-LiteR-specific space to speed up reformulation-based query answering under DL-LiteR constraints. Another difference w.r.t. is that this work explores the usage of DB2’s RDF store, and find it unsuitable to the complex queries resulting from reformulation.

In the database and Semantic Web communities, there have been intense efforts invested in developing scalable RDF data management platforms, including distributed ones; see e.g., the survey. However, these platforms do not take constraints into account, and thus only support query evaluation, not query answering. Our work is the first to consider optimized algorithms for answering queries under DL-LiteR constraints through relational databases.

In the area of cost-based complex query optimization, MQO/CSE algorithms have been described e.g., in. Oracle includes several query rewrites to improve nested query performance, among which subquery coalesce reduces some redundancy and thus can be seen as related to CSE. A different class of techniques improve the performance of multiple concurrent reads of a table: this can be seen as a physical-level MQO only applying to one-table plans. Such techniques are implemented in DB2, and they indeed help evaluating our reformulations. However, as stated in Section, our approach does not require detecting repeated subexpressions.

We plan to extend our framework to efficient query answering using materialized CQ views, which may partially or completely rewrite the CQs appearing in the reformulated fragments.

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8. REFERENCES

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