OBDA Constraints for Effective Query Answering (Extended Version)

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Abstract. In Ontology Based Data Access (OBDA) users pose SPARQL queries over an ontology that lies on top of relational datasources. These queries are translated on-the-fly into SQL queries by OBDA systems. Standard SPARQL-to-SQL translation techniques in OBDA often produce SQL queries containing redundant joins and unions, even after a number of semantic and structural optimizations. These redundancies are detrimental to the performance of query answering, especially in complex industrial OBDA scenarios with large enterprise databases. To address this issue, we introduce two novel notions of OBDA constraints and show how to exploit them for efficient query answering. We conduct an extensive set of experiments on large datasets using real world data and queries, showing that these techniques strongly improve the performance of query answering up to orders of magnitude.

1 Introduction

In Ontology Based Data Access (OBDA) \cite{DBLP:journals/sigmod/Kifer07}, the complexity of data storage is hidden by a conceptual layer on top of an existing relational database (DB). Such a conceptual layer, realized by an ontology, provides a convenient vocabulary for user queries, and captures domain knowledge (e.g., hierarchies of concepts) that can be used to enrich query answers over incomplete data. The ontology is connected to the relational database through a declarative specification given in terms of mappings that relate each term in the ontology (each class and property) to a (SQL) view over the database. The mappings and the database define a (virtual) RDF graph that, together with the ontology, can be queried using the SPARQL query language.

To answer a SPARQL query over the conceptual layer, a typical OBDA system translates it into an equivalent SQL query over the original database. The translation procedure has two major stages: (1) \textit{rewriting} the input SPARQL query with respect to the ontology and (2) \textit{unfolding} the rewritten query with respect to the mappings. A well-known theoretical result is that the size of the translation is worst-case exponential in the size of the input query \cite{DBLP:journals/sigmod/Kifer07}. These worst-case scenarios are not only theoretical, but they also occur in real-world applications, as shown in \cite{DBLP:conf/semweb/HovlandLM16}, where some user SPARQL queries are translated into SQL queries containing thousands of join and union operators. This is mainly due to (i) SPARQL queries containing joins of ontological terms with rich hierarchies, which lead to redundant unions \cite{DBLP:conf/semweb/HovlandLM16}; and (ii) reifications of n-ary relations in the database into triples over the RDF data model, which lead to SQL translations containing several (mostly redundant) self-joins. How to reduce the impact of
exponential blow-ups through optimization techniques so as to make OBDA applicable to real-world scenarios is one of the main open problems in current OBDA research.

The standard solutions to tackle this problem are based on semantic and structural optimizations \[19,20\] originally from the database area \[5\]. Semantic optimizations use explicit integrity constraints (such as primary and foreign keys) to remove redundant joins and unions from the translated queries. Structural optimizations are in charge of reshaping the translations so as to take advantage of database indexes.

The main problem addressed in this paper is that these optimizations cannot exploit constraints that go beyond database dependencies, such as domain constraints (e.g., people have only one age, except for Chinese people who have two ages), or storage policies in the organization (e.g., table married must contain all the married employees). We address this problem by proposing two novel classes of constraints that go beyond database dependencies. The first type of constraint, exact predicate, intuitively describes classes and properties whose elements can be retrieved without the help of the ontology. The second type of constraint, virtual functional dependency (VFD), intuitively describes a functional dependency over the virtual RDF graph exposed by the ontology, the mappings, and the database. These notions are used to enrich the OBDA specification so as to allow the OBDA system to identify and prune redundancies from the translated queries. To help the design of enriched specifications, we provide tools that detect the satisfied constraints within a given OBDA instance. We extend the OBDA system Ontop so as to exploit the enriched specification, and evaluate it in both a large-scale industrial setting provided by the petroleum company Statoil, and in an ad-hoc artificial and scalable benchmark with different commercial and free relational database engines as back-ends. Both sets of experiments reveal a drastic reduction on the size of translated queries, which in some cases is reduced by orders of magnitudes. This allows for a major performance improvement of query answering.

The rest of the paper is structured as follows: Preliminaries are provided in Section\[2\]. In Section\[3\] we describe how state-of-the-art OBDA systems work, and highlight the problems with the current optimization techniques. In Section\[4\] we formally introduce our novel OBDA constraints, and show how they can be used to optimize translated queries. In Section\[5\] we provide an evaluation of the impact of the proposed optimization techniques on the performance of query answering. In Section\[6\] we briefly survey other related works. Section\[7\] concludes the paper. The omitted proofs and extended experiments with Wisconsin benchmark can be found in the appendix.

2 Preliminaries

We assume the reader to be familiar with relational algebra and SQL queries, as well as with ontology languages and in particular with the OWL 2 QL\[1\] profile. To simplify the notation we express OWL 2 QL axioms by their description logic counterpart DL-Lite\[R\] \[4\]. Notation-wise, we will denote tuples with the bold faces; e.g., $x$ is a tuple.

**Ontology and RDF Graphs.** The building block of an ontology is a vocabulary ($N_C, N_R$), where $N_C, N_R$ are respectively countably infinite disjoint sets of class names and (object or datatype) property names. A predicate is either a class name or a property name. An ontology is a finite set of axioms constructed out a vocabulary, and it describes a domain

\[1\] http://www.w3.org/TR/owl2-overview/
of interest. These axioms of an ontology can be serialized into a concrete syntax. In the following we use the Turtle syntax for readability.

Example 1. The ontology from Statoil captures the domain knowledge related to oil extraction activities. Relevant axioms for our examples are:

| Axiom                                      |
|--------------------------------------------|
| :isInWell rdfs:domain :Wellbore             |
| :hasInterval rdfs:domain :Wellbore          |
| :completionDate rdfs:domain :Wellbore       |
| :ProdWellbore rdfs:subClassOf :DevelopWellbore |
| :DevelopWellbore rdfs:subClassOf :Wellbore  |

The first five axioms specify domains and ranges of the properties :isInWell, :hasInterval, and :completionDate. The last two state the hierarchy between different wellbore classes.

Given a countably infinite set \( N_I \) of individual names disjoint from \( N_C \) and \( N_R \), an assertion is an expression of the form \( A(i) \) or \( P(i_1, i_2) \), where \( i, i_1, i_2 \in N_I \), \( A \in N_C \), \( P \in N_R \). An OWL 2 QL knowledge base (KB) is a pair \((T, \mathcal{A})\) where \( T \) is an OWL 2 QL ontology and \( \mathcal{A} \) is a set of assertions (also called ABox). Semantics for entailment of assertions \((\models)\) in OWL 2 QL KBs is given through Tarski-style interpretations in the usual way \[^1\]. Given a KB \((T, \mathcal{A})\), the saturation of \( \mathcal{A} \) with respect to \( T \) is the set of assertions \( \mathcal{A}_T = \{ A(s) \mid (T, \mathcal{A}) \models A(s) \} \cup \{ P(s, o) \mid (T, \mathcal{A}) \models P(s, o) \} \). In the following, it is convenient to view assertions \( A(s) \) and \( P(s, o) \) as the RDF triples \((s, rdf:type, A)\) and \((s, P, o)\), respectively. Hence, we view a set of assertions also as an RDF graph \( G^\mathcal{A} \) defined as \( G^\mathcal{A} = \{(s, rdf:type, A) \mid A(s) \in \mathcal{A}\} \cup \{(s, P, o) \mid P(s, o) \in \mathcal{A}\} \). Moreover, the saturated RDF graph \( G^{(T, \mathcal{A})} \) associated to a knowledge base \((T, \mathcal{A})\) consists of the set of triples entailed by \((T, \mathcal{A})\), i.e. \( G^{(T, \mathcal{A})} = G^\mathcal{A} \).

**OBDA and Mappings.** Given a vocabulary \((N_C, N_R)\) and a database schema \( \Sigma \), a mapping is an expression of the form \( A(f_1(x_1)) \leftarrow sql(y) \) or \( P(f_1(x_1), f_2(x_2)) \leftarrow sql(y) \), where \( A \in N_C \), \( P \in N_R \), \( f_1, f_2 \) are function symbols, \( x_i \subseteq y \) for \( i = 1, 2 \), and \( sql(y) \) is an SQL query in \( \Sigma \) having output attributes \( y \). Given \( Q \) in \( N_C \cup N_R \), a mapping \( m \) is defining \( Q \) if \( Q \) is on the left hand side of \( m \).

Given an SQL query \( q \) and a DB instance \( D \), \( q^D \) denotes the set of answers to \( q \) over \( D \). Given a database instance \( D \) and a set of mappings \( M \), we define the virtual assertions set \( \mathcal{A}_{MD} \) as follows:

\[
\mathcal{A}_{MD} = \{ A(f(o)) \mid o \in \pi_x(sql(y))^D \text{ and } A(f(x)) \leftarrow sql(y) \text{ in } M \} \cup \{ P(f(o), g(o')) \mid (o, o') \in \pi_{x,x}(sql(y))^D \text{ and } P(f(x_1), g(x_2)) \leftarrow sql(y) \text{ in } M \}
\]

In the Turtle syntax for mappings, we use templates—strings with placeholders—for specifying the functions (like \( f \) and \( g \) above) that map database values into URIs and literals. For instance, the string \(<http://statoil.com/[id]>\) is a URI template where “id” is an attribute; when \( id \) is instantiated as “1”, it generates the URI \(<http://statoil.com/1>\).

An OBDA specification is a triple \( S = (T, M, \Sigma) \) where \( T \) is an ontology, \( \Sigma \) is a database schema with key dependencies, and \( M \) is a set of mappings between \( T \) and \( \Sigma \). Given an OBDA specification \( S \) and a database instance \( D \), we call the pair \((S, D)\) an OBDA instance. Given an OBDA instance \( O = ((T, M, \Sigma), D) \), the virtual RDF graph

\(^2\) A wellbore is a three-dimensional representation of a hole in the ground.
exposed by $O$ is the RDF graph $G^{\mathcal{A}_{MD}}$; the saturated virtual RDF graph $G^{O}$ exposed by $O$ is the RDF graph $G^{(T,\mathcal{A}_{MD})}$.

**Example 2.** The mappings for the classes and properties introduced in Example 1 are:

```
:Wellbore-[wellbore,a] rdf:type :Wellbore
← SELECT wellbore FROM wellbore WHERE wellbore.r.existence[kd]nm = 'actual'

:Wellbore-[wellbore,a] :isInWell :Well-[well,a]
← SELECT wellbore, well FROM wellbore WHERE wellbore.r.existence[kd]nm = 'actual'

:Wellbore-[wellbore,a] :hasInterval :WellboreInterval-[wellbore-intv,a]
← SELECT wellbore, wellbore-intv FROM wellbore_interval

:Wellbore-[wellbore,a] :completionDate ['year']-[month]-[day]'ˆˆxsd:date
← SELECT wellbore, year, month, day FROM wellbore WHERE wellbore.r.existence[kd]nm = 'actual'

:Wellbore-[wellbore,a] rdf:type :ProdWellbore
← SELECT w.wellbore AS wellbore FROM wellbore w, facility[clsn] WHERE complex-expression
```

**Query Answering in OWL 2 QL KBs.** A conjunctive query $q(x)$ is a first order formula of the form $\exists y. \varphi(x, y)$, where $\varphi(x, y)$ is a conjunction of equalities and atoms of the form $A(t), P(t_1, t_2)$ (where $A \in N_C, P \in N_R$), and each $t, t_1, t_2$ is either a term or an individual variable in $x, y$. Given a conjunctive query $q(x)$ and a knowledge base $\mathcal{K} := (T, \mathcal{A})$, a tuple $i \in N^\mathcal{I}$ is a certain answer to $q(x)$ iff $\mathcal{K} \models q(i)$. The task of query answering in OWL 2 QL (DL-Lite$\mathcal{Q}$) can be addressed by query rewriting techniques [14]. For an OWL 2 QL ontology $T$, a conjunctive query $q$ can be rewritten to a union $q_f$ of conjunctive queries such that for each assertion set $\mathcal{A}$ and each tuple of individuals $i \in N^\mathcal{I}$, it holds $(T, \mathcal{A}) \models q(i) \Rightarrow \mathcal{A} \models q_f(i)$. Many rewriting techniques have been proposed in the literature [14][23].

SPARQL [9] is a W3C standard language designed to query RDF graphs. Its vocabulary contains four pairwise disjoint and countably infinite sets of symbols: $I$ for IRIs, $B$ for blank nodes, $L$ for RDF literals, and $V$ for variables. The elements of $C = I \cup B \cup L$ are called RDF terms. A triple pattern is an element of $(C \cup V) \times I \times (C \cup V)$. A basic graph pattern (BGP) is a finite set of joins of triple patterns. BGPs can be combined using the SPARQL operators join, optional, filter, projection, etc.

**Example 3.** The following SPARQL query, containing a BGP with three triple patterns, returns all the wellbores, their completion dates, and the well where they are contained.

```
SELECT * WHERE (?wlb rdf:type:Wellbore. ?wlb:completionDate ?cmpl. ?wlb:isInWell ?w.)
```

To ease the presentation of the technical development, in the rest of this paper we adopt the OWL 2 QL entailment regime for SPARQL query answering [15], but disallow complex class/property expressions in the query. Intuitively this restriction states that each BGP can be seen as a conjunctive query without existentially quantified variables. Under this restricted OWL 2 QL entailment regime, the task of answering a SPARQL query $q$ over a knowledge base $(T, \mathcal{A})$ can be reduced to answering $q$ over the saturated graph $G^{(T,\mathcal{A})}$ under the simple entailment regime. This restriction can be lifted with the help of a standard query rewriting step [15].
3 SPARQL Query Answering in OBDA

In this section we describe the typical steps that an OBDA system performs to answer SPARQL queries and discuss the performance challenges. To do so, we pick the representative state-of-the-art OBDA system Ontop and discuss its functioning in detail.

During its start-up, Ontop classifies the ontology, "compiles" the ontology into the mappings generating the so-called \( T \)-mappings [19], and removes redundant mappings by using inclusion dependencies (e.g., foreign keys) contained in the database schema. Intuitively, \( T \)-mappings expose a saturated RDF graph. Formally, given a basic OBDA specification \( S = (T, M, \Sigma) \), the mappings \( M_T \) are \( T \)-mappings for \( S \) if, for every OBDA instance \( O = (S, D) \), \( G_O = G^{(A_{MT}, D)} \).

Example 4. The \( T \)-mappings for our running example are those in Example 2 plus:

\[
:Wellbore\{wellbore\} rdf:type :Wellbore \leftarrow \text{SELECT wellbore\_s FROM wellbore WHERE wellbore\_r\_existence\_kd\_nm = 'actual'}
\]

\[
:Wellbore\{wellbore\} rdf:type :Wellbore \leftarrow \text{SELECT wellbore\_s, wellbore\_intv\_s FROM wellbore\_interval}
\]

\[
:Wellbore\{wellbore\} rdf:type :Wellbore \leftarrow \text{SELECT w.wellbore\_s FROM wellbore w, facility\_clsn WHERE ... complex-expression}
\]

The new mappings are derived from the domain of the properties :isInWell, :completionDate, and because :ProdWellbore is a sub-class of :Wellbore.

After the start-up, in the query answering stage, Ontop translates the input SPARQL query into an SQL query, evaluates it, and returns the answers to the end-user. We divide this stage in five phases: (a) the SPARQL query is rewritten using the tree-witness rewriting algorithm; (b) the rewritten SPARQL query is unfolded into an SQL query using \( T \)-mappings; (c) the resulting SQL query is optimized; (d) the optimized SQL query is executed by the database engine; (e) the SQL result is translated into the answer to the original SPARQL query. For the sake of simplicity, we disregard phase (a) since it goes out of the scope of this paper (cf. [10]), and phases (d) and (e) because they are straightforward. In the following we elaborate on phases (b) and (c).

From SPARQL to SQL. In phase (b) the rewritten SPARQL query is unfolded into an SQL query using \( T \)-mappings. The rewritten query is first transformed into a tree representation of its SPARQL algebra expression. The algorithm starts by replacing each leaf of the tree, that is, a triple pattern of the form \((s, p, o)\), with the union of the SQL queries defining \( p \) in the \( T \)-mapping. Such SQL queries are obtained as follows: given a triple pattern \( p = ?x rdf:type :A \), and a mapping \( m = :A(f(y')) \leftarrow sql(y) \), the SQL unfolding \( \text{unf}(p, m) \) of \( p \) by \( m \) is the SQL query \text{SELECT } \tau(f(y')) \text{ AS } x \text{ FROM } sql(y) \), where \( \tau \) is an SQL function filling the placeholders in \( f \) with values in \( y' \). We denote the sub-expression "\text{SELECT } \tau(f(y')) \text{ AS } x" by \( \pi_{x/f(y')} \). The notions of "\text{unf}" and "\( \pi \)" are defined similarly for properties.

Example 5. Consider the triple pattern \( p = ?wb :completionDate ?d \) and the fourth mapping \( m \) from Example 2. Then the SQL unfolding \( \text{unf}(p, m) \) is the SQL query:

\[
\text{SELECT CONCAT("Wellbore-",wellbore\_s) AS wb,CONCAT("\'",year,"-",month,"-",day,"\'\""\"\"xsd:date") AS d FROM wellbore WHERE wellbore\_r\_existence\_kd\_nm = 'actual'}
\]
Given a triple pattern $p$ and a set of mappings $M$, the SQL unfolding $\text{unf}(p, M)$ of $p$ by $M$ is the SQL union $\bigcup_{m \in M} \{ \text{unf}(p, m) | \text{unf}(p, m) \text{ is defined} \}$.

Once the leaves are processed, the algorithm processes the upper levels in the tree, where the SPARQL operators are translated into the corresponding SQL operators (Project, InnerJoin, LeftJoin, Union, and Filter). Once the root is translated the process terminates and the resulting SQL expression is returned.

Example 6. The unfolded SQL query for the SPARQL query in Example 3 and $\mathcal{T}$-mappings in Example 4 has the following shape:

$$(\pi_{\text{wlb}/\text{sql}:\text{Wellbore}} \cup \pi_{\text{wlb}/\text{sql}:\text{ProdWellbore}} \cup \pi_{\text{wlb}/\text{sql}:\text{hasInterval}})$$

$$\bowtie (\pi_{\text{wlb}/\text{sql}:\text{completionDate}}) \bowtie (\pi_{\text{wlb}/\text{sql}:\text{isInWell}})$$

where $\square = \text{:Wellbore\{-wellbore\}_s}$, $\Diamond = \text{\{year\}-\{month\}-\{day\}}\text{-xsd:date}$, $\odot = \text{:Well\{-well\}_s}$, and $\text{sql}_P$ is the SQL query in the mapping defining the class/property $P$.

Optimizing the generated SQL queries. At this point, the unfolded SQL queries are merely of theoretical value as they would not be efficiently executable by any database system. A problem comes from the fact that they contain joins over the results of built-in database functions, which are expensive to evaluate. Another problem is that the unfoldings are usually verbose, often containing thousands of unions and join operators. Structural and semantic optimizations are in charge of dealing with these two problems.

Structural Optimizations. To ease the presentation, we assume the queries to contain only one BGP. Extending to the general case is straightforward. An SQL unfolding of a BGP has the shape of a join of unions $Q = Q_1 \bowtie Q_2 \ldots \bowtie Q_n$, where each $Q_i$ is a union of sub-queries. The first step is to remove duplicate sub-queries in each $Q_i$. In the second step, $Q$ is transformed into a union of joins. In the third step, all joins of the kind $\pi_{x/f/\text{sql}_1}(z) \bowtie \pi_{x/g/\text{sql}_2}(w)$ where $f \neq g$ are removed because they do not produce any answer. In the fourth step, the occurrences of the SQL function $\pi$ for creating URIs are pushed to the root of the query tree so as to obtain efficient queries where the joins are over database values rather than over URIs. Finally, duplicates in the union are removed.

Semantic Optimizations. SQL queries are semantically analyzed with the goal of transforming them into a more efficient form. The analyses are based on database integrity constraints (precisely, primary and foreign keys) explicitly defined in the database schema. These constraints are used to identify and remove redundant self-joins and unions from the unfolded SQL query.

How Optimized are Optimized Queries? There are real-world cases where the optimizations discussed above are not enough to mitigate the exponential explosion caused by the unfolding. As a result, the unfolded SQL queries cannot be efficiently handled by DB engines [16]. However, the same queries can usually be manually formulated in a succinct way by database managers. A reason for this is that database dependencies cannot model certain domain constraints or storage policies that are available to the database manager but not to the OBDA system. The next example, inspired by the Statoil use case explained in Section 5, illustrates this issue.

Example 7. The data stored at Statoil has certain properties that derive from domain constraints or storage policies. Consider a modified version of the query defining the
class :Wellbore where all the attributes are projected out. According to storage policies for the database table wellbore, the result of the evaluation of this query against any database instance must satisfy the following constraints: (i) it must contain all the wellbores in the ontology (modulo templates); (ii) every tuple in the result must contain the information about name, date, and well (no nulls); (iii) for each wellbores in the result, there is exactly one date/well that is tagged as ‘actual’.

Query with Redundant Unions. Consider the SPARQL query retrieving all the wellbores, namely \( \text{SELECT } * \text{ WHERE } \{ ?wlb \text{ rdf:type :Wellbore}. \} \). By ontological reasoning, the query will retrieve also the wellbores that can be inferred from the subclasses of :Wellbore and from the properties where :Wellbore is the domain or range. Thus, after unfolding and optimizations, the resulting SQL query has the structure \( \pi_{\text{wlb/□}}(\text{sql}_1) \), with \( \text{sql}_1 = (\text{sql}_1:\text{Wellbore} \cup \text{sql}_1:\text{ProdWellbore} \cup \pi_{\#}\text{sql}_1:\text{hasInterval}) \), where \( □ = :\text{Wellbore}-\{\text{wellbores}_s\} \), and \( # = \text{wellbores}_s \). However, all the answers returned by \( \text{sql}_1 \) are also returned by the query \( \text{sql}_1:\text{Wellbore} \) alone, when these two queries are evaluated on a data instance satisfying item (i).

Query with Redundant Joins. For the SPARQL query in Example 3, the unfolded and optimized SQL translation is of the form \( \pi_{\text{wlb/□}}(\text{cmp/w}) \), \( \text{cmp/w} \sim \text{sql}_2 \) with \( \text{sql}_2 = \text{sql}_1 \bowtie \text{sql}_1:\text{completionDate} \bowtie \text{sql}_1:\text{isInWell} \). Observe that the answers from \( \text{sql}_2 \) could also be retrieved from a projection and a selection over wellbore. This is because \( \text{sql}_1 \) could be simplified to \( \text{sql}_1:\text{Wellbore} \) and items (ii) and (iii). The problem we highlight here is that this “optimized” SQL query contains two redundant joins if storage policies and domain constraints are taken into account.

It is important to remark that the constraints in the previous example cannot be expressed through schema dependencies like foreign or primary keys (because these constraints are defined over the output relations of SQL queries in the mappings, rather than over database relations). Therefore, current state-of-the-art optimizations applied in OBDA cannot exploit this information.

4 OBDA Constraints

We now formalize two properties over an OBDA instance: exact predicates and virtual functional dependencies. We will then enrich the OBDA specification with a constraints component, stating that all the instances for the specification display such properties. We show how this additional constraint component can be used to identify and remove redundant unions and joins from the unfolded queries.

From now on, let \( O = (S, D) \) be an OBDA instance of a specification \( S = (T, M, \Sigma) \).

4.1 Exact Predicates in an OBDA Instance

In real world scenarios it often happens that axioms in the ontology do not enrich the answers to queries. Often this is due to storage policies not available to the OBDA system. This fact leads to redundant unions in the generated SQL, as shown in Example 7. In this section we show how certain properties defined on the mappings and the

\( ^3 \) i.e., individuals in the class :Wellbore

\( ^4 \) Materializing the SQL in the mappings is not an option, since the schema is fixed.
predicates, ideally deriving from such constraints, can be used to reduce the number of redundant unions in the generated SQL queries for a given OBDA instance.

**Definition 1 (Exact Mapping).** Let $M'$ be a set of mappings defining a predicate $A$. We say that $M'$ is exact for $A$ in $O$ if $O \models A(a)$ if and only if $((\emptyset, M', \Sigma), D) \models A(a)$.

In practice it is often the case that the mappings for a particular predicate declared in the OBDA specification are already exact. This leads us to the next definition.

**Definition 2 (Exact Predicate).** A predicate $A$ is exact in $O$ if the set of all the mappings in $M$ defining $A$ are exact for $A$ in $O$.

Recall that *Ontop* adds new mappings to the initial set of mappings through the $T$-mapping technique. For exact predicates, this can be avoided while producing the same saturated virtual RDF graph. Fewer mappings lead to unfoldings with less unions.

**Proposition 1.** Let $M'$ be exact for the predicate $A$ in $T$. Let $M'_T$ be the result of replacing all the mappings defining $A$ in $M_T$ by $M'$. Then $G^O = G^{((\emptyset, M'_T, \Sigma), D)}$.

**Example 8.** The $T$-mappings for :Wellbore consist of four mappings (see Example 4). However, :Wellbore is an exact class (Example 7). Therefore we can drop the three $T$-mappings for :Wellbore inferred from the ontology, and leave only its original mapping.

### 4.2 Functional Dependencies in an OBDA instance

Recall that in database theory a functional dependency (abbr. FD) is an expression of the form $x \rightarrow y$, read $x$ functionally determines $y$, where $x$ and $y$ are tuples of attributes. We say that $x \rightarrow y$ is over an attributes set $R$ if $x \subseteq R$ and $y \subseteq R$. Finally, $x \rightarrow y$ is satisfied by a relation $I$ on $R$ if $x \rightarrow y$ is over $R$ and for all tuples $u, v \in I$, if the value $u[x]$ of $x$ in $u$ is equal to the value $v[x]$ of $x$ in $v$, then $u[y] = v[y]$. Whenever $R$ is clear from the context, we simply say that $x \rightarrow y$ is satisfied in $I$.

A virtual functional dependency intuitively describes a functional dependency on a saturated virtual RDF graph. We identify two types of virtual functional dependencies:

- **Branching VFD:** This dependency describes the relation between an object and a set of functional properties providing information about this object. Intuitively, it corresponds to a “star” of “functional-like” properties in the virtual RDF graph. For instance, given a person, the properties describing its (unique) gender, national id, biological mother, etc. are a branching VFD.

- **Path VFD:** This dependency describes the case when, from a given individual and a list of properties, there is at most one path that can be followed using the properties in the list. For instance, $x$ works in a single department $y$, and $y$ has a single manager $w$, and $w$ works for a single company $z$.

We use these notions to identify those cases where a SPARQL join of properties translates into a redundant SQL join.

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5 A property which is functional when restricting its domain/range to individuals generated from a single template.
Definition 3 (Virtual Functional Dependency). Let $t$ be a template, and $s_t$ be the set of individuals in $G^O$ generated from $t$. Let $P, P_1, \ldots, P_n$ be properties in $T$. Then

- A branching VFD is an expression of the form $t \mapsto^{b} P_1 \cdots P_n$. A VFD $t \mapsto^{b} P$ is satisfied in $O$ if for each element $s \in s_t$, there are no $o \neq o'$ in $G^O$ such that $(s, P, o), (s, P, o') \subseteq G^O$. A VFD $t \mapsto^{b} P_1 \cdots P_n$ is satisfied in $O$ if $t \mapsto^{b} P_i$ is satisfied in $O$ for each $i \in \{1, \ldots, n\}$.

- A path VFD is an expression of the form $t \mapsto^{p} P_1 \cdots P_n$. A VFD $t \mapsto^{p} P_1 \cdots P_n$ is satisfied in $O$ if for each $s \in s_t$ there is at most one list of nodes $(o_1, \ldots, o_n)$ in $G^O$ such that $[(s, P, o_1), \ldots, (o_{n-1}, P_n, o_n)] \subseteq G^O$.

The next example shows, similarly as in [23], that general path VFDs cannot be expressed as a combination of path VFDs of length 1.

Example 9. Let $G^O = \{(s, P, o_1), (o_1, P, o_2), (s, P, o'_1)\}$, and $t$ a template such that $s_t = \{s\}$. Then, $t \mapsto^{p} P_1 P_2$ is clearly satisfied in $O$. However, $t \mapsto^{p} P_1$ is not.

A property $P$ might not be functional, but still $t \mapsto^{b} P$ might be satisfied in $O$ for some $t$.

Example 10. Let $G^O = \{(s, P, o_1), (s, P, o_2), (s', P, o_3)\}$, and $t$ a template such that $s_t = \{s'\}$. Then, the VFD $t \mapsto^{p} P$ is satisfied in $O$, but $P$ is not functional.

A functional dependency satisfied in the virtual RDF graph might not correspond to a functional dependency over the database relations. We show this with an example:

Example 11. Consider the following instance of the view wellbore.

| wellbore_s | year | month | day | r_existence | kd | num | well_s |
|-----------|------|-------|-----|-------------|----|-----|-------|
| 002       | 2010 | 04    | 01  | historic    | 1  |     |       |
| 002       | 2009 | 04    | 01  | actual      | 1  |     |       |

The mapping defining :completionDate (c.f. Example 2) uses the view wellbore and has a filter r_existence_kd(num='actual'). Observe that there is no FD (wellbore_s → year month day). However, the VFD :Wellbore-01 :completionDate is satisfied with this data instance, since in $G^O$ the wellbore :Wellbore-002 is connected to a single date "2010-04-01" as a :xsd:date through :completionDate.

Functional dependencies satisfied in a database instance often do not correspond to any VFD at the virtual level. We show this with an example:

Example 12. Consider the table $T_1(x, y, z)$ with a single tuple: $(1, 2, 3)$. Clearly $x \rightarrow y$ and $x \rightarrow z$ are FDs satisfied in $T_1$. Now consider the following mappings:

| [x] | [y] | FROM | T1   | [x] | [z] | FROM | T1   |
|-----|-----|------|------|-----|-----|------|------|

Clearly, there is no VFD involving $P_1$.

Hence, the shape of the mappings affects the satisfiability of VFDs. Moreover, the ontology can also affect satisfiability. We show this with an example:
Example 13. Consider again the data instance $D_E$ from Example 12 and the mappings $M_E$

| $\{x\}$ | $P_1$ | $\{y\} \leftarrow \text{SELECT} \ast \text{ FROM } T_1$ | $\{x\}$ | $P_2$ | $\{z\} \leftarrow \text{SELECT} \ast \text{ FROM } T_1$ |
|-----|-----|------------------|-----|-----|------------------|

Consider an OBDA instance $O_E = ((\emptyset, M_E, T_E) D_E)$. Then the virtual functional dependencies $:i \mapsto b$ $P_1$ and $:i \mapsto b$ $P_2$ are satisfied in $O$. Consider another OBDA instance $O'_E = ((T_E, M_E, \Sigma_E), D_E)$, where $T_E = \{ P_1 \text{ rdfs:subClassOf} P_2 \}$. Then the two VFDs above are not satisfied in $O'_E$.

**VFD Based Optimization** In this section we show how to optimize queries using VFDs. Due to space limitations, we focus on branching VFDs. The results for path VFDs are analogous and can be found in the appendix, as well as proofs.

**Definition 4.** The set of mappings $M$ is basic for $T$ if, for each property $P$ in $T$, $P$ is defined by at most one mapping in $M_T$. We say that $O$ is basic if $M$ is basic for $T$.

To ease the presentation, from now on we assume $O$ to be basic. We denote the (unique) mapping for $P_i$ in $T$, $i \in \{1, \ldots, m\}$, as

$$\hat{t}_d^i(x) \quad P_i \quad \hat{t}_l(y) \leftarrow \text{sql}(z),$$

where $\hat{t}_d^i$ and $\hat{t}_l$ are templates for the domain and range of $P_i$, and $x_i$, $y_i$ are lists of attributes in $z$. The list $z_i$ is the list of projected attributes, which we assume to be the maximal list of attributes that can be projected from sql.

Although we only consider basic instances, we show in the appendix how the results from this section can also be applied to the general case.

We also assume that queries sql$(z_i)$ always contain a filter expression of the form $\sigma_{\text{notNull}(x, y)}$, even if we do not specify it explicitly in the examples, since URIs cannot be generated from nulls [6]. Without loss of generality, we assume that $z_i$ contains all the attributes in $x_1, y_1, \ldots, y_n$.

In order to check satisfiability for a VFD in an OBDA instance one can analyze the DB based on the mappings and the ontology. The next lemma formalizes this intuition.

**Lemma 1.** Let $P_1, \ldots, P_n$ be properties in $T$ such that, for each $1 \leq i < n$, $\hat{t}_d^i = \hat{t}_d^j$. Then, the VFD $\hat{t}_d^i \mapsto b P_1 \ldots P_n$ is satisfied in $O$ if and only if, for each $1 \leq i \leq n$, the FD $x_i \rightarrow y_i$ is satisfied on sql$(z_i)$.

**Example 14.** Consider the properties $:\text{inWell}$ and $:\text{completionDate}$ from our running example. The lemma above suggests that the VFD $:\text{Wellbore}[:i] \mapsto b :\text{inWell}$ is satisfied in our OBDA instance with a database instance $D$ if and only if (i) wellbore$\leftrightarrow$well is satisfied in sql$^D_{:\text{inWell}}$, and (ii) wellbore$\leftrightarrow$year month day is satisfied in sql$^D_{:\text{completionDate}}$.

From Example 12, there is an organization constraint for the view wellbore forcing only one completion date for each “actual” wellbore. As a consequence, the two FDs (i) and (ii) hold in any database $D$ following this organization constraint. Therefore, the VFD in such instance is also satisfied.

We now show how VFDs can be used to find redundant joins that can be eliminated in the SQL translations.
Definition 5 (Optimizing Branching VFD). Let \( t \) be a template. An optimizing branching VFD is an expression of the form \( t \Rightarrow^b P_1 \cdots P_n \). An optimizing VFD \( t \Rightarrow^b P_1 \cdots P_n \) is satisfied in \( O \) if \( t \Rightarrow^b P_1 \cdots P_n \) is satisfied in \( O \), and for each \( i \in \{1, \ldots, n\} \) it holds

\[
\pi_{x_1, y_1, \ldots, y_n}(sql_j(z_i))^D \subseteq \rho_{x_1/n}(\pi_{x_1, y_1, \ldots, y_n}(sql_j(z_i))^D)
\]

(1)

Example 15. Recall that the VFD \( \text{Wellbore}() \Rightarrow^b \text{isInWell}, \text{completionDate} \) is satisfied in our OBDA instance. The precondition (1) holds because (a) the properties are defined by the same SQL query (modulo projection) and (b) the organization constraint “each wellbore entry must contain the information about name, date, and well (no nulls)”. Thus, the optimizing VFD \( \text{Wellbore}() \Rightarrow^D \text{isInWell}, \text{completionDate} \) is satisfied in this instance.

Lemma 2. Consider \( n \) properties \( P_1, \ldots, P_n \) with \( t'_d = t'_p \) for each \( 1 \leq i \leq n \), and for which \( t'_d \Rightarrow^b P_1 \cdots P_n \) is satisfied in \( O \). Then

\[
\pi_\gamma(sql_j(z_i))^D = \pi_\gamma(sql_j(z_i)) \Rightarrow \pi_{x_1, \ldots, x_n}(sql_j(z_i))^D,
\]

where \( \gamma = x_1, y_1, \ldots, y_n \).

We now show how virtual functional dependencies can be used in presence of triple patterns of the form ?x rdf:type C. As for properties, We assume that for each concept \( C_j \) we have a single \( T \)-mapping of the form \( C_j(t'(x)) \leftarrow sql_j(z_i) \).

Definition 6 (Domain Optimizing Class Expression). A domain optimizing class expression (domain OCE) is an expression of the form \( \gamma \Rightarrow^d \rho \), \( C_j \). We say that \( \gamma \Rightarrow^d \rho \), \( C_j \) is satisfied in \( O \) if \( \gamma = \rho \) and \( \pi_\gamma(sql_j(z_i))^D \supseteq \rho_{x_1/n}(\pi_{x_1, y_1, \ldots, y_n}(sql_j(z_i))^D) \).

Definition 7 (Range Optimizing Class Expression). A range optimizing class expression (range OCE) is an expression of the form \( \gamma \Rightarrow^r \rho \), \( C_j \). We say that \( \gamma \Rightarrow^r \rho \), \( C_j \) is satisfied in \( O \) if \( t_j = t'_r \) and \( \pi_\gamma(sql_j(z_i))^D \supseteq \rho_{x_1/n}(\pi_{x_1, y_1, \ldots, y_n}(sql_j(z_i))^D) \).

Optimizing VFDs and classes give us a tool to identify those BGPs whose SQL translation can be optimized by removing redundant joins.

Definition 8 (Optimizable branching BGP). A BGP \( \beta \) is optimizable w.r.t. \( v = t_d \Rightarrow^b P_1 \cdots P_n \) if (i) \( v \) is satisfied in \( O \); (ii) the BGP of triple patterns in \( \beta \) involving properties is of the form \(?v P_1 \ldots ?v P_n \); and (iii) for each triple pattern of the form \(?u rdf:type C in \beta \), \(?u \) is either the subject of some \( P_i \) and \( t'_d \Rightarrow^d \), \( C \) is satisfied in \( O \), or \( ?u \) is in the object of some \( P_i \) and \( t'_r \Rightarrow^r \), \( C \) is satisfied in \( O \).

Finally, we prove that the standard SQL translation of optimizable BGPs contains redundant SQL joins that can be safely removed.

Theorem 1. Let \( \beta \) be an optimizable BGP w.r.t. \( t_d \Rightarrow^x P_1 \cdots P_n \) (\( x = b, p \)) in \( O \). Let \( \pi_{v_1, \ldots, v_n}(sql_\beta)^D = sql_j(x_1, y_1, \ldots, y_n) \). Then \( sql_\beta^D \) and \( sql_\beta'^D \) return the same answers.
Corollary 1. Let $Q$ be a SPARQL query. Let $sql_Q$ be the SQL translation of $Q$ as explained in Section 3. Let $sql'_Q$ be the SQL translation of $Q$ where all the SQL expressions corresponding to an optimizable BGPs w.r.t. a set of VFDs have been optimized as stated in Theorem 1. Then $sql_Q$ and $sql'_Q$ return the same answers.

Example 16. It is clear that the class :Wellbore is optimizing w.r.t. the domain of :completionDate and :isInWell. Since :Wellbore-{}, completionDate, :isInWell is satisfied (c.f. Example 15), one can allow the semantic optimizations to safely remove redundant joins in query $sql_1$, sketched in Example 7. From Theorem 1, it follows that, $sql_{Wellbore} \bowtie sql_{completionDate} \bowtie sql_{isInWell}$ can be by simplified to $sql_{Wellbore}$.

4.3 Enriching the OBDA Specification with Constraints

We propose to enrich the traditional OBDA specification with a constraint component, so as to allow the OBDA system to perform enhanced optimization as described in the previous section. More formally, an OBDA specification with constraints is a tuple $S_{constr} = (S, C)$ where $S$ is an OBDA specification and $C$ is a set of exact mappings, exact predicates, optimizing virtual functional dependencies, and optimizing class expressions. An instance of $S_{constr}$ is an OBDA instance of $S$ satisfying the constraints in $C$. Our intention is to be able to use more of the constraints that exist in real databases for query optimization, since we often see that these cannot be expressed by existing database constraints (i.e. keys). Since $S$ does not necessarily imply $C$, checking the validity of $C$ may have to take into account more information than just $S$. The constraints $C$ may be known to hold e.g. by policy, or be enforced by external tools, e.g., as in the case mentioned in the experiments below, by the tool used to enter data into the database.

In order to aid the user in the specification of $C$, we implemented tools to identify what exact mappings and optimizing virtual functional dependencies are satisfied in a given OBDA instance (see appendix). The user can then verify whether these suggested constraints hold in general, for example because they derive from storage policies or domain knowledge, and provide them as parameters to the OBDA system. The user intervention is necessary, because constraints derived from actual data can be an artifact of the current situation of the database.

Optimizing VFD Constraints. We have implemented a tool that automatically finds a restricted type of optimizing VFDs satisfied in a given OBDA instance and we have extended Ontop to complement semantic optimization using these VFDs. This implementation aims to mitigate the problem of redundant self-joins resulting from reifying relational tables. Although this is a simple case, it is extremely common in practice and, as we show in our experiments in Section 5, this class of VFDs is powerful enough to sensibly improve the execution times in real world scenarios.

Exact Predicates Constraints. We implemented a tool to find exact predicates, and we extended Ontop to optimize $T$-mappings with them. For each predicate $P$ in the ontology $T$ of an OBDA instance $O$, the tool constructs the query $q$ that returns all the individual/pairs in $P$. Then it evaluates $q$ in the two OBDA instances $O$ and ($\emptyset, M, \Sigma, D$). If the answers for $q$ coincide in both instances, then $P$ is exact.
Table 1: Results from the tests over EPDS.

|                      | std. opt | w/VFD | w/both  |
|----------------------|---------|-------|---------|
| Number of queries timing-out | 17      | 10    | 11      |
| Number of fully answered queries | 43      | 50    | 49      |
| Avg. SQL query length (in characters) | 51521   | 28112 | 32364   |
| Average unfolding time | 3.929 s | 3.917 s| 1.142 s |
| Average total query exec. time with timeouts | 376.540 s | 243.935 s | 267.863 s |
| Median total query exec. time with timeouts | 35.241 s | 11.135 s | 21.602 s |
| Average successful query exec. time (without timeouts) | 36.540 s | 43.935 s | 51.217 s |
| Median successful query exec. time (without timeouts) | 12.551 s | 8.277 s | 12.437 s |
| Average number of unions in generated SQL | 6.3      | 4.4    | 5.1     |
| Average total number of tables in generated SQL | 21.0     | 18.2   | 20.0    |

5 Experiments

In this section we present a set of experiments evaluating the techniques described above. In the appendix we ran additional controlled experiments using an OBDA benchmark built on top of the Wisconsin benchmark [7], and obtain similar results to the ones here.

Statoil Scenario In this section we briefly describe the Statoil use-case, and the challenges it presents for OBDA. At Statoil, users access several databases on a daily basis, and one of the most important ones is the Exploration and Production Data Store (EPDS) database. EPDS is a large legacy SQL (Oracle 10g) database comprising over 1500 tables (some of them with up to 10 million tuples) and 1600 views. The complexity of the SQL schema of EPDS is such that it is counter-productive and error-prone to manually write queries over the relational database. Thus, end-users either use only a set of tools with predefined SQL queries to access the database, or interact with IT experts so as to formulate the right query. The latter process can take weeks. This situation triggered the introduction of OBDA in Statoil in the context of the Optique project [13]. In order to test OBDA at Statoil, the users provided 60 queries (in natural language) that are relevant to their job, and that cannot be easily performed or formulated at the moment. The Optique partners formulated these queries in SPARQL, and handcrafted an ontology, and a set of mappings connecting EPDS to the ontology. The ontology contains 90 classes, 37 object properties, and 31 data properties; and there are more than 140 mappings. The queries have between 0 to 2 complex filter expressions (with several arithmetic and string operations), 0 to 5 nested optionals, modifiers such as ORDER BY and DISTINCT; and up to 32 joins.

Experiment Results. The queries were executed sequentially on a HP ProLiant server with 24 Intel Xeon CPUs (X5650 @ 2.67 GHz), 283 GB of RAM. Each query was evaluated three times and we took the average. We ran the experiments with 4 exact concepts and 15 virtual functional dependencies, found with our tools and validated by database experts. The 60 SPARQL queries have been executed over Ontop with and without the optimizations for exact predicates and virtual functional dependencies. We consider that a query times out if the average execution time is greater than 20 minutes.

The results are summarized in Table 1 and Figure 1. We can see that the proposed optimizations allow Ontop to critically reduce the query size and improve the performance of the query execution by orders of magnitude. Specifically, in Figure 1 we compare standard optimizations with and without the techniques presented here. Observe...
that the average successful query execution time is higher with new optimizations than without because the number of successfully executed queries increases. With standard optimizations, 17 SPARQL queries time out. With both novel optimizations enabled, only four queries still time out.

A total of 27 SPARQL queries get a more compact SQL translation with new optimizations enabled. The largest proportional decrease in size of the SQL query is 94\%, from 171\,k\,chars, to 10\,k. The largest absolute decrease in size of the SQL is 408\,k\,chars. Note that the number of unions in the SQL may decrease also only with VFD-based optimization. Since the VFD-based optimization removes joins, more unions may become equivalent and are therefore removed. The maximum measured decrease in execution time is on a query that times out with standard optimizations, but uses 3.7 seconds with new optimizations.

6 Related work

Dependencies have been intensively studied in the context of traditional relational databases \[2\]. Our work is related to the one in \[23\]; in particular their notion of path functional dependency is close to the notion of path VFD presented here. However, they do not consider neither ontologies, nor databases, and their dependencies are not meant to be used to optimize queries. There are a number of studies on functional dependencies in RDF \[24\,11\], but as shown in Example \[12\] functional dependencies in RDF do not necessarily correspond to a VFD (when considering the ontology). Besides, these works do not tackle the issue of SQL query optimization.

The notion of perfect mapping \[8\] is strongly related to the notion of exact mapping. However there is a substantial difference: a perfect mapping must be entailed by the OBDA specification, whereas exact mappings are additional constraints that enrich the OBDA specification. For instance, perfect mappings would not be effective in the Statoil use case, where organizational constraints and storage policies are not entailed by the OBDA specification. The notion of EBox \[21\,17\] was proposed as an attempt to include constraints in OBDA. However, EBox axioms are defined through a $\mathcal{T}$-box like syntax. These axioms cannot express constraints based on templates like virtual functional dependencies.

7 Conclusions

In this work we presented two novel optimization techniques for OBDA that complement standard optimizations in the area, and enable efficient SPARQL query answering over enterprise relational data. We provided theoretical foundations for these techniques
based on two novel OBDA constraints: virtual functional dependencies, and exact predicates. We implemented these techniques in our OBDA system OnTop and empirically showed their effectiveness through extensive experiments that display improvements on the query execution time up to orders of magnitude.

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A Appendix

A.1 Background On SPARQL to SQL

In this section, we recap the complete SPARQL to SQL translation [15]. This background will be used for the proofs in the following sections.

SPARQL under Simple Entailment SPARQL is a W3C standard language designed to query RDF graphs. Its vocabulary contains four pairwise disjoint and countably infinite sets of symbols: I for IRIs, B for blank nodes, L for RDF literals, and V for variables. The elements of \( C = I \cup B \cup L \) are called RDF terms. A triple pattern is an element of \((C \cup V) \times (I \cup V) \times (C \cup V)\). A basic graph pattern (BGP) is a finite set of triple patterns. Finally, a graph pattern, \( P \), is an expression defined by the grammar

\[
P := \text{BGP} \mid \text{Filter}(P,F) \mid \text{Bind}(P,v,c) \mid \text{Union}(P_1,P_2) \mid \text{Join}(P_1,P_2) \mid \text{Ort}(P_1,P_2,F),
\]

where \( F \), a filter, is a formula constructed from atoms of the form \( \text{bound}(v) \), \( (v = c) \), \( (v = v') \), for \( v, v' \in V \), \( c \in C \), and possibly other built-in predicates using the logical connectives \( \land \) and \( \neg \). The set of variables in \( P \) is denoted by \( \text{var}(P) \).

A SPARQL query is a graph pattern \( P \) with a solution modifier, which specifies the answer variables—the variables in \( P \) whose values we are interested in—and the form of the output (we ignore other solution modifiers for simplicity). The values to variables are given by solution mappings, which are partial maps \( s : V \to C \) with (possibly empty) domain \( \text{dom}(s) \). In this paper, we use the set-based (rather than bag-based, as in the specification) semantics for SPARQL. For sets \( S_1 \) and \( S_2 \) of solution mappings, a filter \( F \), a variable \( v \in V \) and a term \( c \in C \), let

- \( \text{Filter}(S,F) = \{ s \in S \mid F^s = \top \} \);
- \( \text{Bind}(S,v,c) = \{ s \in S \mid v \in \text{dom}(s) \land (v \mapsto c) \subseteq s \} \) (provided that \( v \notin \text{dom}(s) \), for \( s \in S \));
- \( \text{Union}(S_1,S_2) = \{ s \in S_1 \cup S_2 \mid s \in S_1 \lor s \in S_2 \} \);
- \( \text{Join}(S_1,S_2) = \{ s \in S_1 \cup S_2 \mid s_1 \in S_1 \land s_2 \in S_2 \; \text{ are compatible} \} \);
- \( \text{Ort}(S_1,S_2,F) = \text{Filter}(\text{Join}(S_1,S_2),F) \cup \{ s \in S_2 \mid \text{ for all } s_2 \in S_2, \text{ either } s_1, s_2 \; \text{are incompatible or } F^{s_1 \oplus s_2} \neq \top \} \).

Here, \( s_1 \) and \( s_2 \) are compatible if \( s_1(v) = s_2(v) \), for any \( v \in \text{dom}(s_1) \cap \text{dom}(s_2) \), in which case \( s_1 \oplus s_2 \) is a solution mapping with \( s_1 \oplus s_2 : v \mapsto s_1(v) \), for \( v \in \text{dom}(s_1) \), \( s_1 \oplus s_2 : v \mapsto s_2(v) \), for \( v \in \text{dom}(s_2) \), and \( \text{domain } (s_1) \cup (s_2) \). The truth-value \( F^s \in \{ \top, \bot, \varepsilon \} \) of a filter \( F \) under a solution mapping \( s \) is defined inductively:

- \( (\text{bound}(v))^s = \top \) if \( v \in \text{dom}(s) \) and \( \bot \) otherwise;
- \( (v = c)^s = \varepsilon \) if \( v \notin \text{dom}(s) \); otherwise, \( (v = c)^s \) is the classical truth-value of the predicate \( s(v) = c \); similarly, \( (v = v')^s = \varepsilon \) if either \( v \) or \( v' \notin \text{dom}(s) \); otherwise, \( (v = v')^s \) is the classical truth-value of the predicate \( s(v) = s(v') \);
- \( (\neg F)^s = \begin{cases} \varepsilon, & \text{if } F^s = \varepsilon, \\ \neg F^s, & \text{otherwise.} \end{cases} \)
- \( (F \land F')^s = \begin{cases} \bot, & \text{if } F_1^s = \bot \text{ or } F_2^s = \bot, \\ \top, & \text{if } F_1^s = F_2^s = \top, \\ \varepsilon, & \text{otherwise.} \end{cases} \)

Here, \( (v = c)^s = \top \) if \( v \in \text{dom}(s) \) and \( \bot \) otherwise.
Finally, given an RDF graph $G$, the answer to a graph pattern $P$ over $G$ is the set $\llbracket P \rrbracket_G$ of solution mappings defined by induction using the operations above and starting from the following base case: for a basic graph pattern $B$,

$$\llbracket B \rrbracket_G = \{ s: \text{var}(B) \to C \mid s(B) \subseteq G \},$$

(2)

where $s(B)$ is the set of triples resulting from substituting each variable $u$ in $B$ by $s(u)$. This semantics is known as simple entailment.

Translating SPARQL under Simple Entailment to SQL We recap the basics of relational algebra and SQL (see e.g., [?]). Let $U$ be a finite (possibly empty) set of attributes. A tuple over $U$ is a map $t: U \to A$, where $A$ is the underlying domain, which always contains a distinguished element $\text{null}$. A $(|U|\text{-ary})$ relation over $U$ is a finite set of tuples over $U$ (again, we use the set-based rather than bag-based semantics). A filter $F$ over $U$ is a formula constructed from atoms $\text{isNull}(u')$, $(u = c)$ and $(u = u')$, where $U' \subseteq U$, $u, u' \in U$ and $c \in A$, using the connectives $\land$ and $\neg$. Let $\mathcal{F}$ be a filter with variables $U$ and let $t$ be a tuple over $U$. The truth-value $F' \in \{ \top, \bot, \varepsilon \}$ of $F$ over $t$ is defined inductively:

- $(\text{isNull}(U'))^t = \top$ if $t(u)$ is $\text{null}$, for all $u \in U'$, and $\bot$ otherwise;
- $(u = c)^t = \varepsilon$ if $t(u)$ is $\text{null}$; otherwise, $(u = c)^t$ is the classical truth-value of the predicate $t(u) = c$; similarly, $(u = u')^t = \varepsilon$ if either $t(u)$ or $t(u')$ is $\text{null}$; otherwise, $(u = u')^t$ is the classical truth-value of the predicate $t(u) = t(u')$;
- $(-F)^t = \begin{cases} \varepsilon, \\ \neg F^t, \end{cases}$ if $F^t = \varepsilon$, and $(F_1 \land F_2)^t = \begin{cases} \bot, \\ \top, \end{cases}$ if $F_1^t = \bot$ or $F_2^t = \top$;

(Note that $\neg$ and $\land$ are interpreted in the same three-valued logic as in SPARQL.) We use standard relational algebra operations such as union, difference, projection, selection, renaming and natural (inner) join. Let $R_i$ be a relation over $U_i$, $i = 1, 2$.

- If $U_1 = U_2$ then the standard $R_1 \cup R_2$ and $R_1 \setminus R_2$ are relations over $U_1$.
- If $U \subseteq U_1$ then $\pi_U R_1 = R_1|_U$ is a relation over $U$.
- If $F$ is a filter over $U_1$ then $\sigma_F R_1 = \{ t \in R_1 \mid F^t = \top \}$ is a relation over $U_1$.
- If $v \notin U_1$ and $u \in U_1$ then $\rho_{v/u} R_1 = \{ t_{v/u} \mid t \in R_1 \}$, where $t_{v/u}: v \mapsto t(u)$ and $t_{v/u}: u' \mapsto t(u')$, for $u' \in U_1 \setminus \{ u \}$, is a relation over $(U_1 \setminus \{ u \}) \cup \{ v \}$.
- $R_1 \bowtie R_2 = \{ t_1 \bowtie t_2 \mid t_1 \in R_1 \text{ and } t_2 \in R_2 \text{ are compatible} \}$ is a relation over $U_1 \times U_2$. Here, $t_1$ and $t_2$ are compatible if $t_1(u) = t_2(u) \neq \text{null}$, for all $u \in U_1 \cap U_2$, in which case a tuple $t_1 \bowtie t_2$ over $U_1 \cup U_2$ is defined by taking $t_1 \bowtie t_2: u \mapsto t_1(u)$, for $u \in U_1$, and $t_1 \bowtie t_2: u \mapsto t_2(u)$, for $u \in U_2$ (note that if $u$ is $\text{null}$ in either of the tuples then they are incompatible).

To bridge the gap between partial functions (solution mappings) in SPARQL and total mappings (on attributes) in SQL, we require one more operation (expressible in SQL):

- If $U \cap U_1 = \emptyset$ then the padding $\mu_U R_1$ is $R_1 \bowtie \text{null}^U$, where $\text{null}^U$ is the relation consisting of a single tuple $t$ over $U$ with $t: u \mapsto \text{null}$, for all $u \in U$.  

By an SQL query, $Q$, we understand any expression constructed from relation symbols (each over a fixed set of attributes) and filters using the relational algebra operations given above (and complying with all restrictions on the structure). Suppose $Q$ is an SQL query and $D$ a data instance which, for any relation symbol in the schema under consideration, gives a concrete relation over the corresponding set of attributes. The answer to $Q$ over $D$ is a relation $||Q||_D$ defined inductively in the obvious way starting from the base case: for a relation symbol $Q$, $||Q||_D$ is the corresponding relation in $D$.

We now define a translation, $\tau$, which, given a graph pattern $P$, returns an SQL query $\tau(P)$ with the same answers as $P$. More formally, for a set of variables $V$, let $\text{ext}_{V}$ be a function transforming any solution mapping $s$ with $\text{dom}(s) \subseteq V$ to a tuple over $V$ by padding it with nulls:

$$\text{ext}_{V}(s) = \{ v \mapsto s(v) \mid v \in \text{dom}(s) \} \cup \{ v \mapsto \text{null} \mid v \in V \setminus \text{dom}(s) \}.$$

The relational answer to $P$ over $G$ is $||P||_G = \{ \text{ext}_{\text{var}(P)}(s) \mid s \in ||P||_G \}$. The SQL query $\tau(P)$ will be such that, for any RDF graph $G$, the relational answer to $P$ over $G$ coincides with the answer to $\tau(P)$ over $\text{triple}(G)$, the database instance storing $G$ as a ternary relation $\text{triple}$ with the attributes subj, pred, obj. First, we define the translation of a SPARQL filter $F$ by taking $\tau(F)$ to be the SQL filter obtained by replacing each $\text{bound}(v)$ with $\text{isNull}(v)$ (other built-in predicates can be handled similarly).

**Proposition 2.** Let $F$ be a SPARQL filter and let $V$ be the set of variables in $F$. Then $F^* = (\tau(F))^{\text{ext}_{V}(s)}$, for any solution mapping $s$ with $\text{dom}(s) \subseteq V$.

The definition of $\tau$ proceeds by induction on the construction of $P$. Note that we can always assume that graph patterns under simple entailment do not contain blank nodes because they can be replaced by fresh variables. It follows that a BGP $\{tp_1, \ldots, tp_n\}$ is equivalent to $\text{Join}((tp_1), \text{Join}((tp_2), \ldots))$. So, for the basis of induction we set

$$\tau(\{(s, p, o)\}) =
\begin{cases}
\pi_{\text{subj}}(s) \land \pi_{\text{pred}}(p) \land \pi_{\text{obj}}(o) \text{ triple}, & \text{if } s, p, o \in I \cup L, \\
\pi_{\text{subj}}(s) \land \pi_{\text{pred}}(p) \land \pi_{\text{obj}}(o) \text{ triple}, & \text{if } s \in V \text{ and } p, o \in I \cup L, \\
\pi_{\text{subj}}(s) \land \pi_{\text{pred}}(p) \land \pi_{\text{obj}}(o) \text{ triple}, & \text{if } s, o \in V, s \neq o, p \in I \cup L, \\
\pi_{\text{subj}}(s) \land \pi_{\text{pred}}(p) \land \pi_{\text{obj}}(o) \text{ triple}, & \text{if } s, o \in V, s = o, p \in I \cup L, \\
\vdots
\end{cases}$$

(the remaining cases are similar). Now, if $P_1$ and $P_2$ are graph patterns and $F_1$ and $F$ are filters containing only variables in $\text{var}(P_1)$ and $\text{var}(P_1) \cup \text{var}(P_2)$, respectively, then we set $U_i = \text{var}(P_i)$, $i = 1, 2$, and

$$\begin{aligned}
\tau(\text{Filter}(P_1, F_1)) &= \sigma_{\tau(F_1)}(\tau(P_1)), \\
\tau(\text{Bind}(P_1, v, c)) &= \tau(P_1) \bowtie \{ v \mapsto c \}, \\
\tau(\text{Union}(P_1, P_2)) &= \mu_{U_1 \cup U_2} \tau(P_1) \cup \mu_{U_1 \setminus U_2} \tau(P_2), \\
\tau(\text{Join}(P_1, P_2)) &= \bigcup_{V_1, V_2 \subseteq U_1 \cap U_2} \left[ \left( \sigma_{\tau(P_1) \mid V_1} \sigma_{\text{isNull}(V_1)}(\tau(P_1)) \bowtie \sigma_{\tau(P_2) \mid V_2} \sigma_{\text{isNull}(V_2)}(\tau(P_2)) \right) \right], \\
\tau(\text{Opt}(P_1, P_2, F)) &= \tau(\text{Filter}(\text{Join}(P_1, P_2), F)) \cup \\
&\quad \mu_{U_1 \setminus U_2} \left( \tau(P_1) \setminus \bigcup_{V_1 \subseteq U_1 \cap U_2} \sigma_{\mu_{V_1} \sigma_{\tau(P_2) \mid V_2} \tau(\text{Filter}(\text{Join}(P_1, P_2, F)))} \right),
\end{aligned}$$

for $\mu_{F_1 \setminus F_2}(s) = \{ v \mapsto s(v) \mid v \in F_1 \setminus F_2 \}$.
where \( P^{\mathcal{U}}_V = \text{FILTER}(P, \bigwedge_{v \in V} \neg \text{bound}(v) \land \bigwedge_{v \in V} \text{bound}(v)) \). It is readily seen that any \( \tau(P) \) is a valid SQL query and defines a relation over \( \text{var}(P) \); in particular, \( \tau(\text{Join}(P_1, P_2)) \) is a relation over \( \bigcup_{i=1,2}(U_i \setminus V_i) = U_1 \cup U_2 = \text{var}(\text{Join}(P_1, P_2)) \).

**Theorem 2.** For any RDF graph \( G \) and any graph pattern \( P \), \( ||P||_G = ||\tau(P)||_{\text{tuple}(G)} \).

**R2RML Mappings** The SQL translation of a SPARQL query constructed above has to be evaluated over the ternary relation \( \text{tuple}(G) \) representing the virtual RDF graph \( G \). Our aim now is to transform it to an SQL query over the actual database, which is related to \( G \) by means of an R2RML mapping \([6]\). We begin with a simple example.

**Example 17.** The following R2RML mapping (in the Turtle syntax) populates an object property \( \text{ub:UGDegreeFrom} \) from a relational table \( \text{students} \), whose attributes \( \text{id} \) and \( \text{degreeuniid} \) identify graduate students and their universities:

\[
\_\_m1 \text{ a } \text{rr:TripleMap};
\]

\[
\quad \text{rr:logicalTable} \text{ [ } \text{rr:sqlQuery "SELECT * FROM students WHERE stype=1" ];}
\]

\[
\quad \text{rr:subjectMap} \text{ [ } \text{rr:template "/GradStudent(id)" ];}
\]

\[
\quad \text{rr:predicateObjectMap} \text{ [ } \text{rr:predicate ub:UGDegreeFrom} ;
\]

\[
\quad \quad \text{rr:objectMap} \text{ [ } \text{rr:template "/Uni(degreeuniid)" ] ]}
\]

More specifically, for each tuple in the query, an R2RML processor generates an RDF triple with the predicate \( \text{ub:UGDegreeFrom} \) and the subject and object constructed from attributes \( \text{id} \) and \( \text{degreeuniid} \), respectively, using IRI templates.

Our aim now is as follows: given an R2RML mapping \( M \), we are going to define an SQL query \( \text{tr}_M(\text{triple}) \) that constructs the relational representation \( \text{tuple}(G_{D,M}) \) of the virtual RDF graph \( G_{D,M} \) obtained by \( M \) from any given data instance \( D \). Without loss of generality and to simplify presentation, we assume that each triple map has

- one logical table (\( \text{rr:sqlQuery} \)),
- one subject map (\( \text{rr:subjectMap} \)), which does not have resource typing (\( \text{rr:class} \)),
- and one predicate-object map with one \( \text{rr:predicateMap} \) and one \( \text{rr:objectMap} \).

This normal form can be achieved by introducing predicate-object maps with \( \text{rdf:type} \) and splitting any triple map into a number of triple maps with the same logical table and subject. We also assume that triple maps contain no referencing object maps (\( \text{rr:parentTriplesMap} \), etc.) since they can be eliminated using joint SQL queries \([6]\). Finally, we assume that the term maps (i.e., subject, predicate and object maps) contain no constant shortcuts and are of the form \( [\text{rr:column } v], [\text{rr:constant } c] \) or \( [\text{rr:template } s] \).

Given a triple map \( m \) with a logical table (SQL query) \( R \), we construct a selection \( \sigma_{\neg\text{isNull}(v_1)} \cdots \sigma_{\neg\text{isNull}(v_k)} R \), where \( v_1, \ldots, v_k \) are the referenced columns of \( m \) (attributes of \( R \) in the term maps in \( m \))—this is done to exclude tuples that contain \textit{null} \([6]\). To construct \( \text{tr}_m \), the selection filter is prefixed with projection \( \pi_{\text{subj, pred, obj}} \) and, for each of the three term maps, either with renaming (e.g., with \( \rho_{\text{obj}} \) if the object map is of the form \( [\text{rr:column } v] \)) or with value creation (if the term map is of the form \( [\text{rr:constant } c] \) or \( [\text{rr:template } s] \)) in the latter case, we use the built-in string concatenation function \( \| \). For instance, the mapping \( \_\_m1 \) from Example \([17]\) is converted to the SQL query

\[
\text{SELECT } \text{"\text{\textbackslash /GradStudent\textbackslash /id}" AS subj, \text{"\textbackslash ub:UGDegreeFrom\textbackslash /pred},
\]

\[
\text{\textbackslash /Uni\textbackslash /degreeuniid\textbackslash /obj} \text{ FROM students}
\]

\[
\text{WHERE (id IS NOT NULL) AND (degreeuniid IS NOT NULL) AND (stype=1)}.
\]
Given an R2RML mapping $M$, we set $\text{tr}_M(\text{triple}) = \bigcup_{m \in M} \text{tr}_m$.

**Proposition 3.** For any R2RML mapping $M$ and data instance $D$, $t \in \|\text{tr}_M(\text{triple})\|_D$ if and only if $t \in \text{triple}(G_{D,M})$.

Finally, given a graph pattern $P$ and an R2RML mapping $M$, we define $\text{tr}_M(\tau(P))$ to be the result of replacing every occurrence of the relation triple in the query $\tau(P)$, constructed in Section A.1, with $\text{tr}_M(\text{triple})$. By Theorem 2 and Proposition 3 we obtain:

**Theorem 3.** For any graph pattern $P$, R2RML mapping $M$ and data instance $D$, $\|P\|_{G_{D,M}} = \|\text{tr}_M(\tau(P))\|_D$.

### A.2 Proofs of Section 4.1

**Proposition 1**. Let $M'$ be exact for the predicate $A$ in $\mathcal{T}$. Let $M'_\ell$ be the result of replacing all the mappings defining $A$ in $M_\ell$ by $M'$. Then $G^O = G^{(0,M'_\ell,\ell),D}$.

**Proof (Sketch).** By the definition of $\mathcal{T}$-mappings, we have $G^O = G^{0,M'_\ell,\ell,D}$. For all predicates other than $A$, $M_\ell$ and $M'_\ell$ produce the same set of triples since the mappings defining them are identical. For the predicate $A$, since $M'$ is exact in $O$, $M_\ell$ and $M'_\ell$ also produce same set of triples. Therefore $G^{0,M'_\ell,\ell,D} = G^{0,M_\ell,\ell,D}$.

### A.3 Proofs of Section 4.2

**Lemma 1**. Let $P_1, \ldots, P_n$ be properties in $\mathcal{T}$ such that, for each $1 \leq i < n$, $i \rightarrow i'$ is satisfied in $G^O$ if and only if, for each $1 \leq i \leq n$, the $\text{FD} x_i \rightarrow y_i$ is satisfied on $\text{sql}(z_i)$.

**Proof.**

1. $i \rightarrow i'$ is satisfied in $G^O$
   - (Definition of FD)
   - $\forall s \in S, \forall 1 \leq i \leq n : (s, o) \in P_{i'}^O \land (s, o') \in P_i^O \Rightarrow o = o'$
   - (Mappings assumptions for $P_i$)
   - $\forall 1 \leq i \leq n : \forall u \in \pi_x(\text{sql}(z_i)) : (u, y) \in \pi_y(\text{sql}(z_i)) \Rightarrow y = y'$
   - (Definition of Functional Dependency)
   - $\forall 1 \leq i \leq n : y \rightarrow y_i$ is satisfied in $\pi_{y_i}(\text{sql}(z_i))$

**Lemma 2**. Consider $n$ properties $P_1, \ldots, P_n$ in $\mathcal{T}$ with $i \rightarrow i'$ for each $1 \leq i \leq n$, and for which $i \rightarrow i'$ is satisfied in $O$. Then

$$\pi_i(\text{sql}(z_i)) = \pi_i(\text{sql}(z_1) \bowtie_{x_1=x_2} \text{sql}(z_2) \bowtie \cdots \bowtie_{x_1=x_n} \text{sql}(z_n)),$$

where $\gamma = x_1, y_1, \ldots, y_n$. 

Proof. The direction \( \subseteq \) of the equality can be obtained easily. Here we prove the direction \( \supseteq \).

Let \( q_{\text{branch}}^D \) denote the right hand side expression in the equality. Assume the containment \( \supseteq \) does not hold. Then, this means there exists a tuple \((s, v_1, \ldots, v_n)\) such that

\[
\neg (u, v_1, \ldots, v_n) \in q_{\text{branch}}^D \quad \text{and} \quad (u, v_1, \ldots, v_n) \notin \pi_{x_1, \ldots, x_n} \sigma_{\text{nullNull}(x_1,y_1)}sql_1(z_1)^D
\]

The above implies that there exists an index \( j, 1 \leq j \leq n \), such that

\[
\neg (u, v_j) \in \pi_{x_1,y_j} q_{\text{branch}}^D \quad \text{and} \quad (u, v_j) \notin \pi_{x_1,y_j} \sigma_{\text{nullNull}(x_1,y_1)}sql_1(z_1)^D
\]

Then, we can distinguish three cases:

1. \( u \notin \pi_{x_1} \sigma_{\text{nullNull}(x_1,y_1)}sql_1(z_1) \).

Then \( u \notin \pi_{x_1} q_{\text{branch}}^D \), hence \((u, v_j) \notin \pi_{x_1,y_j} q_{\text{branch}}^D \); contradiction.

2. \((u, v_j^*) \in \pi_{x_1,y_j} q_{\text{branch}}^D \) hence \((u, v_j) \notin \pi_{x_1,y_j} q_{\text{branch}}^D \); contradiction.

3. \((u, v_j^*) \in \pi_{x_1,y_j} \sigma_{\text{nullNull}(x_1,y_1)}sql_1(z_1)^D \), \( v_j \neq v_j^* \) and not \( v_j \) nor \( v_j^* \) is null.

This violates the hypothesis that \( t_{\text{d}}^i \leadsto \neg \neg \neg \neg P_1 \cdots P_n \) is satisfied in \( O \), because of Lemma [1].

Hence, by contradiction we conclude that the containment \( \supseteq \) must hold.

\[ \square \]

Results and Proofs for PATH VFDs

Lemma 3. Let \( P_1, \ldots, P_n \) be properties in \( T \) such that, for each \( 1 \leq i \leq n \), \( t_r \equiv t_{d_{n-i}} \).

Then, the VFD \( t_{\text{d}}^i \leadsto \neg \neg \neg \neg P_1 \cdots P_n \) is satisfied in \( O \) if and only if the FD \( x_1 \rightarrow y_1 \cdots y_n \) is satisfied in:

\[
\pi_{x_1,y_1,\ldots,y_n} (sql_1(z_1)) \ni y_1 := x_2 \quad sql_2(z_2) \ni y_2 := x_3 \quad \cdots \quad sql_n(z_n) \ni y_n := x_n
\]

Proof.

\( t_{\text{d}}^i \leadsto \neg \neg \neg \neg P_1 \cdots P_n \) is satisfied in \( G^D \)

\( \uparrow \) (Definition [3])

\( \forall \sigma \in S^1 \cdot \exists (x_1, \ldots, x_n) \in G^D \) such that \((x, P_1, a_1), \ldots, (a_{n-1}, P_n, a_n) \) \( \subseteq G^D \)

\( \uparrow \) (Mappings assumptions for \( P \))

\( \forall u \in \pi_{x_1} \sigma_{\text{nullNull}(x_1,y_1)}sql_1(z_1)^D : \)

\( \forall v_1, v'_1 \in \pi_{x_1} \sigma_{\text{nullNull}(x_1,y_1)}sql_1(z_1)^D : \ldots \forall v_n, v'_n \in \pi_{x_n} \sigma_{\text{nullNull}(x_n,y_n)}sql_n(z_n)^D : \)

\( (u, v_1) \in \pi_{x_1,y_1} \sigma_{\text{nullNull}(x_1,y_1)}sql_1(z_1)^D \land \cdots \land (v_n-1, v_n) \in \pi_{x_{n-1},y_{n-1}} \sigma_{\text{nullNull}(x_{n-1},y_{n-1})}sql_n(z_n)^D \)

\( (u, v'_1) \in \pi_{x_1,y_1} \sigma_{\text{nullNull}(x_1,y_1)}sql_1(z_1)^D \land \cdots \land (v_n-1, v'_n) \in \pi_{x_{n-1},y_{n-1}} \sigma_{\text{nullNull}(x_{n-1},y_{n-1})}sql_n(z_n)^D \Rightarrow v_1 = v'_1 \cdots v_n = v'_n \)
Lemma 3. Proof. (Sketch) The argument is similar to the one of the proof for Lemma 2, by using

\[ (\forall u \in \pi_1(\text{notNull}_{a}), \text{sql}_1(z_1)^D) : \]
\[ \forall v_1, v'_1 \in \pi_1(\text{notNull}_{a}), \text{sql}_1(z_1)^D : \]
\[ (u_1, v_1, \ldots, v_n) \in \pi_{a_1}(\text{notNull}_{a_2}, \text{sql}_2(z_2) \supseteq (\exists v_{a_2}) \text{sql}_{a_2}(z_2) \supseteq (\forall v_{a_3}) \text{sql}_{a_3}(z_2) \supseteq \ldots \supseteq (\forall v_{a_n}) \text{sql}_{a_n}(z_n) \supseteq v'_1, \ldots, v'_n) \]
\[ \text{where } q_1 = v_1, \ldots, v_n = v'_n \]

Definition 10 (Optimizable path BGP). A BGP \( \beta \) is optimizable w.r.t. \( v = t_d \rightsquigarrow P_1 \ldots P_n \) if \( v \) is satisfied in \( O \); (ii) the BGP of triple patterns in \( \beta \) involving properties is of the form \( ?v_0 P_1 ?v_1 \ldots ?v_{n-1} P_n ?v_n \ldots \), and (iii) for every triple pattern of the form \( ?u \text{ rdf:type } C \) in \( \beta \), \( ?u \) is the subject of some \( P_i \) \( (i = 1 \ldots n) \) and \( t_d \rightsquigarrow P_i, C \) is satisfied in \( O \), or \( ?u \) is the object of some \( P_i \) \( (i = 1 \ldots n) \) and \( t_d \rightsquigarrow \text{notNull}_P, C \) is satisfied in \( O \).

Example 18. Consider the following set of \( T \)-mappings for an OBDA setting \( O \):

\[
\begin{align*}
  f(id,name) & \leftarrow \text{SELECT id, name, friend FROM } T \\
g(friend) & \leftarrow \text{SELECT friend, friend_age FROM } T
\end{align*}
\]

Then the lemma above suggests that the VFD \( f \rightsquigarrow P_1 P_2 \) is satisfied in \( O \) if and only if the FD \( id \rightarrow name \) is satisfied in \( (T \rightsquigarrow \text{friend=friend T})^D \).

Definition 9 (Optimizing Path VFD). Let \( t \) be a template, and \( P_1, \ldots, P_n \) be properties in \( T \). An optimizing path VFD is an expression of the form \( t \rightsquigarrow P_1 \ldots P_n \). An optimizing VFD \( t \rightsquigarrow P_1 \ldots P_n \) is satisfied in \( O \) if \( t \rightsquigarrow P_1 \ldots P_n \) is satisfied in \( O \) and

\[
\pi_{x_1y_1 \ldots y_n} \text{sql}_1(z_1)^D \subseteq q_{\text{path}}^D
\]

where

\[
q_{\text{path}} = \pi_{x_1y_1 \ldots y_n} \text{sql}_1(z_1) \supseteq x_1 = x_2, \text{sql}_2(z_2) \supseteq x_2 = x_3, \ldots, \text{sql}_n(z_n).
\]

Lemma 4. Consider \( n \) properties \( P_1, \ldots, P_n \) in \( T \) with \( t_{ri} = t_{di}, \) for each \( 1 \leq i < n, \) and for which \( t_{ri}' \rightsquigarrow P_1 \ldots P_n \) is satisfied in \( O \). Then

\[
\pi_{x_1y_1 \ldots y_n} \text{sql}_1(z_1)^D = q_{\text{path}}^D
\]

where \( q_{\text{path}} \) is the same as in the Definition 9.

Proof. (Sketch) The argument is similar to the one of the proof for Lemma 2 by using Lemma 3.
Proofs for Main Results

Theorem 1. Let $\beta$ be an optimizable BGP w.r.t. $t_d \rightsquigarrow^x P_1 \ldots P_n$ ($x = b, p$) in $O$. Let $\pi_{v_1/v_1, y_1/y_1, \ldots, y_n/y_n} sql_\beta$ be the SQL translation of $\beta$ as explained in Section 3. Let $sql_{\beta}^P = sql_1(x_1, y_1 \ldots y_n)$. Then $sql_{\beta}^P$ and $sql_{\beta}^P$ return the same answers.

Proof. Assume that $t_d \rightsquigarrow^P P_1 \ldots P_n$. The proof for branching functional dependencies is analogous.

From the definition of $\tau$ for triple pattern and the definition of the $\tau$ for $\mathcal{M}$ for BGP$s$ it follows that the BGP $\beta$ will be translated as:

\[
(\pi_{v_0,v_1} \rho_{v_1/\text{subj}} \rho_{v_1/\text{obj}} \sigma_{\text{pred}=P_1 \text{triple}}) \\
\upharpoonright_{v_1=v_2} \\
\vdots \\
\upharpoonright_{v_{n-2}=v_{n-1}} \\
(\pi_{v_{n-1},v_n} \rho_{v_n/\text{subj}} \rho_{v_n/\text{obj}} \sigma_{\text{pred}=P_n \text{triple}})
\]

The table triple is replaced by the definition of the triple patterns in the mappings as follows:

\[
(\pi_{v_0,v_1} \rho_{v_1/\text{subj}} \rho_{v_1/\text{obj}} \sigma_{\text{pred}=P_1 \text{triple}}) (sql_1(z_1)) \\
\upharpoonright_{v_1=v_2} \\
\vdots \\
\upharpoonright_{v_{n-2}=v_{n-1}} \\
(\pi_{v_{n-1},v_n} \rho_{v_n/\text{subj}} \rho_{v_n/\text{obj}} \sigma_{\text{pred}=P_n \text{triple}}) (sql_n(z_n))
\]

This expression can be simplified to:

\[
(\pi_{v_0,v_1} \rho_{v_0/\text{subj}} \rho_{v_1/\text{obj}} \pi_{\text{subj}/y_j, \text{obj}/y_j} \sigma_{\text{pred}=P_1 \text{triple}}) (sql_1(z_1)) \\
\upharpoonright_{v_1=v_2} \\
\vdots \\
\upharpoonright_{v_{n-2}=v_{n-1}} \\
(\pi_{v_{n-1},v_n} \rho_{v_n/\text{subj}} \rho_{v_n/\text{obj}} \pi_{\text{subj}/y_j, \text{obj}/y_j} \sigma_{\text{pred}=P_n \text{triple}}) (sql_n(z_n))
\]

By definition we know that the template in the range of $P_{i-1}$ coincide with the template in $P_i$. Thus, we can remove them from the join over $u_i$'s in (??) and make the join over the attributes $x_i, y_i$ instead of the URIs. Therefore, $\beta$ can be rewritten to

\[
\pi_{v_0/v_1, y_1/y_2, \ldots, y_n/y_n} (sql_1(z_1) \bowtie_{y_1=x_2} sql_2(z_2) \bowtie_{y_2=x_3} \cdots \bowtie_{y_{n-1}=x_n} sql_n(z_n))
\]

(7)

Since $\beta$ is optimizable, we know that

\[
\pi_{x_1,y_1,y_n} sql_1(z_1) = \pi_{x_1,y_1,y_n} (sql_1(z_1) \bowtie_{y_1=x_2} sql_2(z_2) \bowtie_{y_2=x_3} \cdots \bowtie_{y_{n-1}=x_n} sql_n(z_n))
\]

(8)

Therefore, we can simplify (7) to $\pi_{v_0/v_1, y_1/y_2, \ldots, y_n/y_n} (sql_1(z_1))$. This proves the Theorem. \qed
A.4 Lifting Basic OBDA Instance Assumption

We show that the “basic OBDA instance assumption” in Section 4.2 is not a real restriction. A SPARQL query over a $T$-mapping with predicates of multiple templates can be rewritten to another SPARQL query over another $T$-mapping with predicates of only single template.

As usual, we assume an OBDA instance $((\mathcal{T}, \mathcal{M}, \Sigma), D)$, and let $\mathcal{M}_T$ be a $T$-mapping.

Suppose a predicate $A$ is defined by $k$ mapping assertions using different template in $\mathcal{M}_T$:

$$
A(t^1_d(x), t^1_i(y)) \leftrightarrow sql_1(z) \\
\ldots
$$

$$
A(t^k_d(x), t^k_i(y)) \leftrightarrow sql_k(z)
$$

Define $\mathcal{M}'_T$ be the mapping obtained by replacing the assertions for the $A$ with the following $k$ mapping assertions defining $k$ fresh predicates $A_i$ ($i = 1, \ldots, k$):

$$
A_1(t^1_d(x), t^1_i(k(y)) \leftrightarrow sql_1(z) \\
\ldots
$$

$$
A_k(t^k_d(x), t^k_i(y)) \leftrightarrow sql_k(z)
$$

Suppose that $Q$ is a SPARQL query using predicate $A$. The idea is to construct another SPARQL query $Q'$ such that $\llbracket Q \rrbracket_{(\mathcal{M}_T, D)} = \llbracket Q' \rrbracket_{(\mathcal{M}'_T, D)}$. The construction is performed on each triple pattern using $A$. Suppose $B$ is a triple pattern occurring in $Q$; we take $B^+$ to be the union of

$$
B[A \mapsto A_i], \quad i = 1 \ldots k
$$

where $B[A \mapsto A_i]$ is a triple pattern obtained by replacing all the occurrences of $A$ in $B$ with $A_i$. Finally $Q'$ is defined as the SPARQL query obtained by replacing all the triple patterns $B$ with $B^+$.

**Lemma 5.** $\llbracket B \rrbracket_{(\mathcal{M}_T, D)} = \llbracket B^+ \rrbracket_{(\mathcal{M}'_T, D)}$

**Proof.** We only prove the case where $B$ is a single triple pattern of the form $B = (?x, \text{rdf:type}, A)$, since the case where $A$ is a property can be proved analogously. In this case,

$$
B^+ = (?x, \text{rdf:type}, A_1) \cup \ldots \cup (?x, \text{rdf:type}, A_k)
$$

Suppose that $[?x \mapsto a]$ is a solution mapping, i.e., $A(a)$ is in the RDF graph exposed by $\mathcal{M}_T$ and $D$. It follows that there is a mapping assertion $A(t(x)) \leftrightarrow sql_i(z) \in \mathcal{M}_T$, such that $a = t(x_0)$ for some template $t_0$ and tuple $x_0$. Since $A_i(t(x)) \leftrightarrow sql_i(z) \in \mathcal{M}'_T$, we have $A_i(t(x_0))$ is in the RDF graph exposed by $\mathcal{M}'_T$ and $D$. Then $[x \mapsto a]$ is a solution mapping of $(?x, \text{rdf:type}, A_i)$ and also of $B^+$.

The other direction can be proved analogously.

**Theorem 4.** $\llbracket Q \rrbracket_{(\mathcal{M}_T, D)} = \llbracket Q' \rrbracket_{(\mathcal{M}'_T, D)}$

**Proof.** The proof is a standard induction over the structure of the SPARQL queries. The base case of proof is the triple pattern case, and has been proved in Lemma 5. The inductive case can be proved easily.

By exhaustingly apply Theorem 4 to all predicates of different templates, one can lift the restriction of “basic OBDA instance”.

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**OBDA Constraints for Effective Query Answering (Extended Version) 25**

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A.5 Wisconsin Benchmark

We setup an environment based on the Wisconsin Benchmark [7]. This benchmark was designed for the systematic evaluation of database performance with respect to different query characteristics. The benchmark comes with a schema that is designed so one can quickly understand the structure of each table and the distribution of each attribute value. This allows easy construction of queries that isolate the features that need to be tested. The benchmark also comes with a data generator to populate the schema. Unlike EPDS, the benchmark database contains synthetic data that allows easily specifying a wide range of retrieval queries. For instance, in EPDS it is very difficult to specify a selection query with a 20% or 30% selectivity factor. This task becomes even harder when we include joins into the picture.

The benchmark defines a single table schema (which can be used to instantiate multiple tables). The table, which we now call “Wisconsin table”, contains 16 attributes, and a primary key (un.ique2) with integers from 0 to 100 million randomly ordered.

We refer the reader to [7] for details on the algorithm that populates the schema.

Dataset We used Postgres 9.1, and DB2 9.7 as Ontop backends. The query optimizers were left with the default configurations. All the table statistics were updated.

For each DB engine we created a database, each with 10 tables: 5 Wisconsin tables (Tabi, i = 1, . . . , 5), and 5 tables materializing the join of the former tables. For instance, view123 materializes the join of the tables Tab1, Tab2, and Tab3. Each table contains 100 million rows, and each of the databases occupied ca. 400GB of disk space.

Hardware We ran the experiments in an HP Proliant server with 24 Intel Xeon CPUs (@3.47GHz), 106GB of RAM and five 1TB 15K RPM HD. Ontop was run with 6GB Java heap space. The OS is Ubuntu 12.04 LTS 64-bit edition.

In these experiments, we ran each query 3 times, and we averaged the execution times. There was a warm-up phase, where we ran 4 random queries not belonging to the tests.

Evaluating the Impact of VFD-based Optimization The experiments in this section measure the impact of optimization based on VFDs. Optimizations based on branching VFDs and path VFDs produce the same effect in the resulting SQL query, therefore, for concreteness we focus on branching VFD. The performance gain for path VFD is similar.

Recall that we started studying this scenario because EPDS contains thousands of views that lack primary/foreign keys, and some of them cannot be avoided in the mappings. This prevents OBDA semantic optimizations to take place.

The following experiments evaluate the trade-off of using views or their definitions depending on: (i) type of mappings (using views or view definitions); (ii) the complexity of the user query (# of SPARQL joins); (iii) the complexity of the mapping definition (# of SQL joins); (iv) the selectivity of the query; (v) the VFD optimization ON/OFF; (vi) the DB engine (DB2/PostgreSQL);

In the following we describe the queries, mappings and the OBDA specifications and instances used in the different experiments.
Queries In this experiment we tested a set of 36 queries each varying on: (i) the number of SPARQL joins (1-3), (ii) SQL joins in the mappings (1-4), and (iii) selectivity of the query (3 different values). The SPARQL queries have the following shape:

```
SELECT ?x ?y WHERE {
  ?x a :Class-n-SQLs . ?x :Property1-n-SQLs ?y1 .
  .
  .
  .
  ?x :Propertym-n-SQLs ?ym . Filter( ?ym < k% )
}
```

where Class-n-SQLs and Propertyi-n-SQLs are classes and properties defined by mappings which source is either an SQL join of n = 1...4 tables, or a materialized view of the join of n tables. Subindex m represents the number of SPARQL joins, 1 to 3. Regarding the selectivity of k%, we did the experiments with the following values: (i) 0.0001% (100 results); (ii) 0.01% (10,000 results); (iii) 0.1% (100,000 results). These queries do not belong to the Wisconsin benchmark.

OBDA Specifications We have two OBDA settings, one where classes and properties are populated using an SQL that use original tables with primary keys (1-4 joins) (K_1); and a second one where predicates are populated using materialized views (materializing 1-4 joins). This second setting we tested with VFD optimization (K_2) and without optimization (K_3). In the first OBDA setting, all the property subjects are mapped into the tables primary keys. There are no axioms in the ontology. All the individuals have the same template t.

Let S_t be the set of all individuals. In K_2 there are 12 branching VFDs of the form

\[ S_t \rightarrow^b :Property_{m-n-SQLs} \text{ for every } n = 1...4, m = 1...3. \]

The optimizable VFDs contain intuitively the properties populated from the same view, that is,

\[ S_t \rightarrow^b :Property_{1-n-SQLs}, :Property_{2-n-SQLs}, :Property_{3-n-SQLs} \text{ for } n = 1...4. \]

Discussion and Results The results of the experiments are shown in Figure 2. Each q_{i,j} represents the query with i SPARQL joins over properties mapped to j SQL joins.

There is almost no difference between the results with different selectivity, so for clarity we averaged the run times over different selectivities. Since the experiment was run three times, each point in the figure represents the average of 9 query executions.

The experiment results in Figure 2 show that all the SPARQL queries perform better in K_2 than in K_3 in both DB engines. Moreover, in all cases queries in K_2 perform at least twice as fast as the ones in K_3, even getting close to the performance of K_1.

In Ontop-Postgres, the execution of the hardest SPARQL queries in K_1 is 1 order of magnitude faster than in K_2. The execution of these queries in K_2 is 4 times faster than in K_1. In Ontop-DB2, the performance gap between the SPARQL queries in K_3 and K_2 is smaller. The SPARQL queries in K_1 are slightly faster than the queries in K_2. The execution in K_2 is 2 times faster than in K_3.

In Ontop-Postgres and Ontop-DB2, the translations of the SPARQL queries resulting from the K_3 scenario contain self-joins of the non-indexed views that force the DB engines to create hash tables for all intermediate join results which increases the start-up cost of the joins, and the overall execution time. One can observe that in both, Ontop-Postgres and Ontop-DB2, the number of SPARQL joins strongly affect the performance of the query in K_3. In both cases, the SPARQL queries in K_2, because of our
Optimization technique, get translated into a join-free SQL query that requires a single sequential scan of the unindexed view. However, the cost of scanning the whole view to perform a non-indexed filter is still higher than the cost of joins (nested joins in both) of the indexed tables in $K_1$.

**Evaluating the Impact of Exact Mappings** In this test we evaluate the exact mapping optimization technique described in Section 4.1. This experiment is inspired by the use case in EPDS where optimization based on exact mapping can help. The following experiments evaluate the impact of the optimization depending on: (i) the complexity of the query (# of SPARQL joins); (ii) the selectivity of the query; (iii) the number of specified exact classes; (iv) the DB engine (DB2/PostgreSQL).

In the following we describe the tables, ontology, mappings, queries and exact predicate specifications used in the experiment.

**OBDA Specifications** The ontology contains four classes $A_1, A_2, A_3, A_4$, one object property $R$ and one data property $S$. The classes form a hierarchy

$$A_1 \text{ rdfs:subClassOf } A_2, \ A_2 \text{ rdfs:subClassOf } A_3, \ A_3 \text{ rdfs:subClassOf } A_4.$$  

The mappings for classes $A_i$ ($i = 1, \ldots, 4$) are defined over the primary key of Tab$_i$ with different filters, in such a way that each $A_i$ is exact. The mappings for $R$ and $S$ are defined over the primary key column and another unique column (unique1) of Tab$_3$.

**Queries** In this experiment we tested 6 queries ($q_1, \ldots, q_6$) varying on: (i) the number of classes and properties in the SPARQL (1-3) and (ii) the classes used in the query. For instance, $q_3$ is
Exact Concepts We consider the following four exact concept specifications: $E_0 = \emptyset$, $E_1 = \{A_1, A_2\}$, $E_2 = \{A_1, A_2, A_3\}$, $E_3 = \{A_1, A_2, A_3, A_4\}$. Observe that $E_0$ corresponds to the case where no exact mapping optimization is applied.

Discussion and Results The results of the experiments are shown in Figure 3. The results show that the exact mapping optimization improves the performance of all SPARQL queries in both database engines. In particular, under the full optimization setting $E_3$, none of the queries time out (20 mins), and the hardest queries perform orders of magnitude faster than in $E_0$ and even $E_1$.

The performance gain is the result of the elimination of redundant unions. For instance, under $E_0$, SPARQL query $q_3$ is translated into a SQL query with 12 unions, but 11 of them are redundant; applying $E_3$ removes all the redundant unions.
A.6 Experiments Material and Tools

All the material related to the Wisconsin experiment, as well as the tools used to find exact mappings and virtual functional dependencies, can be found on

https://github.com/ontop/ontop-examples/tree/master/ruleml-2016