Selective and Compact Explanations for Negative Answers of Ontology-mediated Queries

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Abstract. Explanations for ontology-mediated query answering, especially for negative answers, have received much interest, yet several challenges remain in their computation and application. One challenge is how to properly handle null values (place-holders) in the explanations, and another challenge is how to compactly represent explanations when a large number of individual constants are involved. In this paper, we propose a new framework that allows users to distinguish abstract explanations (with nulls) from concrete explanations (with constants), which extends existing notions of query abduction. We also introduce a compact representation of explanations as rules. The computation of explanations and their rule representations can utilise efficient query rewriting algorithms. A prototype system is implemented and experimental results show that our system can scale over large datasets, and the number of explanations can be significantly reduced in most cases.

1 Introduction

Ontology-mediated query answering (OQA) has drawn intensive interest [8, 2], where an ontology $\mathcal{O}$ provides a virtual schema to the dataset $\mathcal{D}$ for querying. Various formalisms have been proposed as ontology languages, and in this paper, we consider existential rules (a.k.a. Datalog± and tuple generating dependencies) [1, 7], a family of expressive rule languages that covers Datalog and the underlying formalisms of OWL 2 profiles [6]. Moreover, efficient OQA systems have been developed [7, 15, 3, 17, 21]. Explanation of OQA answers, especially for negative answers, has also been studied [9, 12, 22, 4, 10, 11]. In particular, the explanation of negative answers can be formulated as an abduction problem [5, 9]. The query abduction problem considers an *observation*, which can be expressed as a Boolean query q, and searches for all possible *explanations* as (minimal) sets of facts $\mathcal{E}$ that, together with $\mathcal{O}$ and $\mathcal{D}$, can derive q.

It is shown that query explanation is challenging, as the computational complexity of query explanation is indeed higher than query answering [9]. Also, different from traditional abduction, query explanations may allow place-holders, expressed as nulls, that can be substituted with constants. To illustrate why nulls

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are needed and the challenge that comes with allowing nulls, we use a running example on contact tracing. Consider an ontology $\mathcal{O}$ with three rules:

$$\begin{aligned}
&\mathit{high_risk}(x) \leftarrow \mathit{contact}(x,y), \mathit{high_risk}(y).\\
&\mathit{high_risk}(x) \leftarrow \mathit{visit}(x,y), \mathit{hotspot}(y).\\
&\exists y.\big[\mathit{contact}(x,y) \land \mathit{infected}(y)\big] \leftarrow \mathit{infected}(x).
\end{aligned}$$

The first two rules say someone is considered of high-risk if the person had close contact with another high-risk person or visited a hotspot area. The third rule is an existential rule, saying if someone is infected then the person must had close contact with another infected person. Consider the dataset $\mathcal{D} = \{\mathit{contact}(\mathit{Alice}, p_1), \ldots, \mathit{contact}(\mathit{Alice}, p_n)\}$, which says Alice had close contact with the following persons $p_1, \ldots, p_n$. Now, suppose we have an observation that Alice is of high-risk, that is, we have the observation $q : \mathit{high\_risk}(\mathit{Alice})$, which cannot be derived from existing knowledge $\mathcal{O}$ and $\mathcal{D}$ (hence, q as a Boolean query gets a negative answer). The following explanations exist, $\mathcal{E}_i = \{\mathit{high\_risk}(p_i)\}$ ($1 \leq i \leq n$), which says one of Alice's close-contact persons is high-risk. Another explanation is also plausible, $\mathcal{E}_u = \{\mathit{visit}(\mathit{Alice}, u), \mathit{hotspot}(u)\}$, where u is a null, and it says Alice visited some hotspot area. Such an explanation cannot be expressed without introducing nulls as place-holders.

We note that $\mathcal{E}_u$ and $\mathcal{E}_i$ convey very different information, in the sense that the former essentially represents an abstract pattern of explanations with substitutable values, while the latter are concrete ones referring to specific individuals. It is hard to tell in general which kind of explanations would be better. In some cases, a user may prefer concrete explanations to abstract ones; for instance, to trace high-risk individuals like in $\mathcal{E}_i$. In other cases, a user may have the opposite preference; for instance, to know Alice is high-risk due to visiting *some* hotspots as in $\mathcal{E}_u$. Existing approaches only allow one type of explanations or mix the abstract and concrete explanations. Hence, it is important to introduce a new framework that allows preferences to be specified over the two types of explanations. Furthermore, in the case where concrete explanations $\mathcal{E}_i$'s are preferred, computing all such explanations involves repetitive processes and can be computational expensive, especially when n is huge. More importantly, the size of all generated explanations can be too large for human comprehension. Thus, a compact representation of such explanations is desired.

The contributions of the paper can be summarised as follows. We propose a novel notion of selective explanations, which generalises the existing explanations and allows customised preferences between abstract and concrete explanations. Instead of simply allowing or disallowing nulls, our framework is general and allows preferences to be specified in a more fine-grained manner. We also introduce a rule representation for selective explanations, which can significantly reduce the size of explanations and can be computed efficiently. We present methods for computing selective explanations based on query rewriting for existential rules. Finally, we implement a prototype system, and our experimental evaluation shows our system can scale over very large datasets.

2 Preliminary

Let C, V, N be mutually disjoint infinite sets of constants, variables, and labelled nulls respectively. We use labelled nulls as place-holders in facts that can be substituted by constants or other null values, and a *term* is either a constant, or a variable, or a labelled null. We assume standard first-order logic notions, such as predicates, atoms, formulas and entailment ($\models$). Given a formula φ, we use $\mathsf{C}(\varphi)$, $\mathsf{V}(\varphi)$, $\mathsf{N}(\varphi)$ to denote the set of constants, variables, and labelled nulls occurring in φ respectively, which naturally extend to sets of formulas. For convenience of discussion, we assume each formula employs a distinct set of variables and nulls. A *fact* is an atom whose terms are from $\mathsf{C} \cup \mathsf{N}$, which is seen as a special formula, while a *ground fact* is a fact whose terms are from C only. A *dataset* is a finite set of ground facts. A *signature* is a finite set of predicates, and for a formula φ, $\mathsf{sig}(\varphi)$ denotes the set of predicates occurring in φ, which also extend to sets of formulas. For a signature Σ, $\Phi|_\Sigma$ consists of all the formulas in Φ over Σ.

A *substitution* is a function $\sigma : \mathsf{V} \cup \mathsf{N} \to \mathsf{C} \cup \mathsf{V} \cup \mathsf{N}$. By $t\sigma = t'$, we denote that $t \in \mathsf{V} \cup \mathsf{N}$ is mapped to $t' \in \mathsf{C} \cup \mathsf{V} \cup \mathsf{N}$ by σ. It can be conveniently expressed as a (possibly empty) set $\sigma = \{t_1/t'_1, \ldots, t_n/t'_n\}$ by assuming $t_i\sigma = t'_i$ for $1 \leq i \leq n$ and $t\sigma = t$ for $t \in \mathsf{V} \cup \mathsf{N}$ with $t \neq t_i$; and for a subset of terms $T \subseteq \{t_1, \ldots, t_n\}$, $\sigma|_T$ denotes the substitution $\{t \mapsto t' \in \sigma \mid t \in T\}$. For an atom $P(t_1, \ldots, t_n)$, $P(t_1, \ldots, t_n)\sigma$ denotes the atom $P(t_1\sigma, \ldots, t_n\sigma)$, and it naturally extends to sets of atoms and formulas. For two substitutions σ and γ, their composition is the substitution $\sigma\gamma$ such that $t(\sigma\gamma) = (t\sigma)\gamma$ for each $t \in \mathsf{V} \cup \mathsf{N}$. A *renaming* is a substitution σ satisfying that $t\sigma \in \mathsf{V}$ (or $t\sigma \in \mathsf{N}$) whenever $t \in \mathsf{V}$ (resp., $t \in \mathsf{N}$), and $t\sigma \neq t'\sigma$ for each pair of distinct terms $t \neq t'$. Given two sets of atoms $\mathcal{A}$ and $\mathcal{A}'$, a *homomorphism* from $\mathcal{A}$ to $\mathcal{A}'$ is a substitution σ such that $\mathcal{A}\sigma \subseteq \mathcal{A}'$. We denote $\mathcal{A} \preceq_h \mathcal{A}'$ if there is a homomorphism from $\mathcal{A}$ to $\mathcal{A}'$. Particularly, we say $\mathcal{A}$ and $\mathcal{A}'$ are *equivalent*, denoted $\mathcal{A} \equiv \mathcal{A}'$, if $\mathcal{A} \preceq_h \mathcal{A}'$ and $\mathcal{A}' \preceq_h \mathcal{A}$. Two sets Ξ and Ξ' of atom sets are *equivalent*, denoted $\Xi \equiv \Xi'$, if for each atom set $\mathcal{A} \in \Xi$ there exists an atom set $\mathcal{A}' \in \Xi'$ such that $\mathcal{A} \equiv \mathcal{A}'$, and vice versa.

An *existential rule* (or a rule) r is a formula of the form

$$\forall \vec{x}.\forall \vec{y}.[\exists \vec{z}.\varphi(\vec{x}, \vec{z}) \leftarrow \psi(\vec{x}, \vec{y})]$$

where $\vec{x}$, $\vec{y}$ and $\vec{z}$ are pairwise disjoint vectors of variables, and $\varphi(\vec{x}, \vec{z})$ and $\psi(\vec{x}, \vec{y})$ are conjunctions of atoms whose variables are from respectively $\vec{x} \cup \vec{z}$ and $\vec{x} \cup \vec{y}$. Formula φ is the *head* of the rule r, denoted $\mathsf{head}(r)$, and formula ψ is the *body* of r, denoted $\mathsf{body}(r)$; for notational simplicity, we sometimes use them to represent the set of atoms in the formulas. For brevity, universal quantifiers in a rule are often omitted, and we may express conjunctions using commas.

A *conjunctive query* (CQ) is a first-order formula $q(\vec{x})$ of the form $\exists \vec{y}.\varphi(\vec{x}, \vec{y})$ with $\varphi(\vec{x}, \vec{y})$ being a conjunction of atoms whose variables are from $\vec{x} \cup \vec{y}$. Variables in $\vec{x}$ are *answer variables*, and when $\vec{x}$ is empty the query is Boolean, called a *Boolean conjunctive query* (BCQ) and denoted q. As CQ answering can be reduced to that of BCQs, we will focus on BCQs in this paper. It is often convenient to consider a BCQ as the set of atoms in it.

A *query abduction problem* (*QAP*) [9] is a tuple $\Lambda = (\mathcal{O}, \mathcal{D}, q, \Sigma)$, where $\mathcal{O}$ is a set of existential rules, $\mathcal{D}$ is a dataset, q is a BCQ called the *observation*, and Σ is a set of predicates called the *abducibles*. An *explanation* to Λ is a finite set of facts $\mathcal{E}$ such that $\mathsf{sig}(\mathcal{E}) \subseteq \Sigma$, $\mathcal{O} \cup \mathcal{D} \cup \mathcal{E} \models q$. Note that the consistency condition is omitted from the original definition in [9], as we do not consider constraints (or negation) in the ontologies, yet constraints can be easily added to our approach with additional steps of consistency checking.

3 Selective Explanations

For a QAP, often a large portion of explanations contain redundant information and thus are not suitable for query explanation. Hence, existing query explanation approaches typically adopt some minimality conditions, which are specified through preference relations over explanations [9, 12]. A simple condition is subset minimality (up to renaming). For two sets of facts $\mathcal{E}, \mathcal{E}'$, $\mathcal{E} \preceq_m \mathcal{E}'$ if there exists a renaming of nulls σ such that $\mathcal{E}\sigma \subseteq \mathcal{E}'$. To compactly express multiple explanations of the same patterns using a single representative, another preference is proposed in [12] via the homomorphism relations $\preceq_h$; in particular, $\mathcal{E} \preceq_h \mathcal{E}'$ if there is a substitution σ such that $\mathcal{E}\sigma \subseteq \mathcal{E}'$. In the running example, let all the predicates be abducibles. Besides $\mathcal{E}_i$'s and $\mathcal{E}_u$, $\mathcal{E}_v = \{\mathit{visit}(\mathit{Alice}, v), \mathit{hotspot}(u), \mathit{hotspot}(v)\}$ and $\mathcal{E}_c = \{\mathit{visit}(\mathit{Alice}, c), \mathit{hotspot}(c)\}$ are both explanations, with v being a null and c being a constant. Then, $\mathcal{E}_u \preceq_m \mathcal{E}_v$ and not vice versa. Also, $\mathcal{E}_u \preceq_h \mathcal{E}_c$ and not vice versa.

In what follows, we introduce a novel preference relation for selective explanations (over concrete or abstract explanations) based on a fine-grained partition of abducibles. For a QAP with abducibles Σ, a *selection condition* is a tripartition $S = (\Sigma_C, \Sigma_A, \Sigma_M)$ of Σ (i.e., $\Sigma = \Sigma_C \cup \Sigma_A \cup \Sigma_M$ and $\Sigma_C, \Sigma_A, \Sigma_M$ mutually disjoint), where Σ_C, Σ_A and Σ_M are called *concrete*, *abstract* and *mixed* abducibles, respectively. Intuitively, S specifies that for (parts of) explanations on predicates in Σ_C, constants (i.e., concrete individuals) are preferred over nulls in the explanations; whereas for those on predicates in Σ_A, it is the other way round, and nulls (i.e., place-holders) are preferred over constants. On Σ_M, there is no preference between nulls and constants. To achieve this, we define a preference over explanations such that an explanation $\mathcal{E}$ is preferred if nulls in the atoms over Σ_C are substituted with constants, whereas nulls are preserved in the atoms over Σ_A.

For two explanations $\mathcal{E}$ and $\mathcal{E}'$ to Λ, $\mathcal{E} \preceq_S \mathcal{E}'$ if there exists a substitution σ such that (i) $\mathcal{E}|_{\Sigma_C} \subseteq \mathcal{E}'|_{\Sigma_C}\sigma$, (ii) $\mathcal{E}|_{\Sigma_A}\sigma \subseteq \mathcal{E}'|_{\Sigma_A} \cup \mathcal{D}$, and (iii) $\mathcal{E}|_{\Sigma_M}\sigma \subseteq \mathcal{E}'|_{\Sigma_M}$. Informally, the definition says that $\mathcal{E}$ is at least as preferred as $\mathcal{E}'$ if (i) on the signature Σ_C, $\mathcal{E}$ can be obtained by substituting nulls in $\mathcal{E}'$ and eliminating redundant atoms; and (ii) on the signature Σ_A, $\mathcal{E}$ preserves substitutable nulls that can be mapped to constants in $\mathcal{E}'$ or $\mathcal{D}$. The reason why the condition requires a union with $\mathcal{D}$ can be see in the example below. Finally, condition (iii) says that the preference coincides with $\preceq_h$ (which is stronger than $\preceq_m$) on Σ_M.

Example 1. Consider the running example and let $S = (\{\mathit{high\_risk}, \mathit{contact}\}, \{\mathit{visit}, \mathit{hotspot}\}, \emptyset)$, which means explanations about concrete individuals are preferred on $\{\mathit{high\_risk}, \mathit{contact}\}$, and abstract explanations are preferred on $\{\mathit{visit}, \mathit{hotspot}\}$.

Consider two explanations $\mathcal{E}_1 = \{\mathit{high\_risk}(p_1)\}$ and $\mathcal{E}_v = \{\mathit{contact}(\mathit{Alice}, v), \mathit{high\_risk}(v)\}$ with v being a null. There is a substitution $\sigma = \{v/p_1\}$ satisfying conditions (i) – (iii) for $\mathcal{E}_1 \preceq_S \mathcal{E}_v$, and one can verify that $\mathcal{E}_v \not\preceq_S \mathcal{E}_1$. Intuitively, $\mathcal{E}_1$ is preferred as it reveals a concrete high-risk person.

Suppose $\mathcal{D}$ contains an additional fact $\mathit{hotspot}(\mathit{CBD})$. For another two explanations $\mathcal{E}_u = \{\mathit{visit}(\mathit{Alice}, u), \mathit{hotspot}(u)\}$ and $\mathcal{E}_c = \{\mathit{visit}(\mathit{Alice}, \mathit{CBD})\}$, there exists a substitution $\sigma = \{u/\mathit{CBD}\}$ satisfying $\mathcal{E}_u|_{\Sigma_A}\sigma \subseteq \mathcal{E}_c|_{\Sigma_A} \cup \mathcal{D}$. That is, conditions (i) – (iii) hold for $\mathcal{E}_u \preceq_S \mathcal{E}_c$, and $\mathcal{E}_c \not\preceq_S \mathcal{E}_u$. Intuitively, $\mathcal{E}_u$ is preferred as it provides a high-level explanation, without referring to specific hotspots. It also shows why condition (ii) needs to refer to $\mathcal{D}$.

Based on the new preference relation, we define a general notion of selective explanations.

Definition 1. *Given a QAP Λ and a selection condition S, a* selective explanation *$\mathcal{E}$ to Λ w.r.t. S (or simply S-*explanation*) is an explanation to Λ s.t.*

(1) for each explanation $\mathcal{E}'$ to Λ, if $\mathcal{E}' \preceq_m \mathcal{E}$ then $\mathcal{E} \preceq_m \mathcal{E}'$;
(2) for each explanation $\mathcal{E}'$ to Λ satisfying (1), if $\mathcal{E}' \preceq_h \mathcal{E}$ then $\mathcal{E} \preceq_h \mathcal{E}'$;
(3) for each explanation $\mathcal{E}'$ to Λ satisfying (1) and (2), if $\mathcal{E}' \preceq_S \mathcal{E}$ then $\mathcal{E} \preceq_S \mathcal{E}'$.

$\mathsf{exp}_S(\Lambda)$ *denotes the set of all the S-explanations to Λ.*

Note that conditions (1) and (2) are necessary, as otherwise in Example 1, a non-minimal explanation $\mathcal{E}_1' = \{\mathit{contact}(\mathit{Alice}, p_1), \mathit{high\_risk}(p_1)\}$ would be preferred over the explanation $\mathcal{E}_v = \{\mathit{contact}(\mathit{Alice}, v), \mathit{high\_risk}(v)\}$ as $\mathcal{E}_1' \preceq_S \mathcal{E}_v$.

The explanations defined in [12] only satisfies conditions (1) and (2), which does not allow users to specify, for instance, the preference between $\mathcal{E}_u$ and $\mathcal{E}_c$ in Example 1. As explanations satisfying only conditions (1) and (2) do not distinguish abducibles in Σ, we call them *Σ-explanations* and $\mathsf{exp}_\Sigma(\Lambda)$ denotes the set of all the Σ-explanations to Λ. Our definition coincides with that in [12] when $S = (\emptyset, \emptyset, \Sigma)$, and hence ours is more general. In practice, the selection condition can be determined by the users based on the explanation needs, and the study of suitable selection conditions is out of the scope of this paper. In the reminder of this section, we discuss some properties of the preference relation $\preceq_S$.

First of all, the preference relation $\preceq_S$ is reflexive and transitive.

Lemma 1. *For a QAP Λ and a selection condition S, the relation $\preceq_S$ is a preorder.*

Proof For reflexivity, we want to show for each explanation $\mathcal{E}$ to Λ, $\mathcal{E} \preceq_S \mathcal{E}$. Let σ be the empty substitution (mapping each term to itself), then $\mathcal{E}|_{\Sigma_C} = \mathcal{E}|_{\Sigma_C}\sigma$, $\mathcal{E}|_{\Sigma_A}\sigma \subseteq \mathcal{E}|_{\Sigma_A} \cup D$, and $\mathcal{E}|_{\Sigma_M}\sigma \subseteq \mathcal{E}|_{\Sigma_M}$, that is, $\mathcal{E} \preceq_S \mathcal{E}$.

For transitivity, we assume w.l.o.g. that each explanation have a distinct set of nulls. We want to show for explanations $\mathcal{E}, \mathcal{E}', \mathcal{E}''$ to Λ, if $\mathcal{E} \preceq_S \mathcal{E}'$, $\mathcal{E}' \preceq_S \mathcal{E}''$ then $\mathcal{E} \preceq_S \mathcal{E}''$. From Condition (i), there exist substitutions σ, σ' such that $\mathcal{E}|_{\Sigma_C} \subseteq \mathcal{E}'|_{\Sigma_C}\sigma$, and $\mathcal{E}'|_{\Sigma_C} \subseteq \mathcal{E}''|_{\Sigma_C}\sigma'$. Then, $\mathcal{E}'|_{\Sigma_C}\sigma \subseteq \mathcal{E}''|_{\Sigma_C}\sigma'\sigma$, and $\mathcal{E}|_{\Sigma_C} \subseteq \mathcal{E}''|_{\Sigma_C}\sigma'\sigma$. From Condition (ii), $\mathcal{E}|_{\Sigma_A}\sigma \subseteq \mathcal{E}'|_{\Sigma_A} \cup D$ and $\mathcal{E}'|_{\Sigma_A}\sigma' \subseteq \mathcal{E}''|_{\Sigma_A} \cup D$. Then, $\mathcal{E}|_{\Sigma_A}\sigma\sigma' \subseteq (\mathcal{E}'|_{\Sigma_A} \cup D)\sigma' = \mathcal{E}'|_{\Sigma_A}\sigma' \cup D$, and $\mathcal{E}|_{\Sigma_A}\sigma\sigma' \subseteq \mathcal{E}''|_{\Sigma_A} \cup D$. From Condition (iii), $\mathcal{E}|_{\Sigma_M}\sigma \subseteq \mathcal{E}'|_{\Sigma_M}$, and $\mathcal{E}'|_{\Sigma_M}\sigma' \subseteq \mathcal{E}''|_{\Sigma_M}$. Then, $\mathcal{E}'|_{\Sigma_M}\sigma\sigma' \subseteq \mathcal{E}''|_{\Sigma_M}\sigma'$, and $\mathcal{E}|_{\Sigma_M}\sigma\sigma' \subseteq \mathcal{E}''|_{\Sigma_M}$. Let σ'' be a substitution such that $\sigma''|_{\mathsf{V}(\mathcal{E})} = \sigma\sigma'|_{\mathsf{V}(\mathcal{E})}$ and $\sigma''|_{\mathsf{V}(\mathcal{E}'')} = \sigma'\sigma|_{\mathsf{V}(\mathcal{E}'')}$. We have $\mathcal{E}|_{\Sigma_C} \subseteq \mathcal{E}''|_{\Sigma_C}\sigma''$, $\mathcal{E}|_{\Sigma_A}\sigma'' \subseteq \mathcal{E}''|_{\Sigma_A} \cup D$, and $\mathcal{E}|_{\Sigma_M}\sigma'' \subseteq \mathcal{E}''|_{\Sigma_M}$; that is, $\mathcal{E} \preceq_S \mathcal{E}''$. ∎

Next, the determination of the preference relation between two explanations is NP-complete, which can be proved by a straightforward reduction from the homomorphism problem.

Lemma 2. *For two explanations $\mathcal{E}$ and $\mathcal{E}'$ to a QAP Λ and a selection condition S, deciding whether $\mathcal{E} \preceq_S \mathcal{E}'$ is NP-complete.*

Proof For the membership, a substitution σ guess non-deterministically and condition (i), (ii) and (iii) can be checked in polynomial time.

For the hardness, we show that the homomorphism problem, i.e., whether a set of atoms $\mathcal{A}$ can be homomorphically mapped to another set of atoms $\mathcal{A}'$, which is NP-complete, can be reduced to the decision problem of $\mathcal{A} \prec_S \mathcal{A}'$. We construct a QAP $\Lambda = (\mathcal{O}, \mathcal{D}, q, \Sigma)$, where $\mathcal{O} = \{Q \leftarrow \bigwedge \mathcal{A}, Q \leftarrow \bigwedge \mathcal{A}'\}$ where Q is a nullary atom, $\mathcal{D} = \emptyset$, $q = Q$, and $\Sigma = \mathsf{sig}(\mathcal{A} \cup \mathcal{A}')$. Then, clearly $\mathcal{A}$ and $\mathcal{A}'$ are both explanations to Λ. Take a selection condition $S = (\emptyset, \emptyset, \Sigma)$. According to the definition of $\preceq_S$, there is a homomorphism from $\mathcal{A}$ to $\mathcal{A}'$, i.e., $\mathcal{A}\sigma \subseteq \mathcal{A}'$ for some substitution σ, iff $\mathcal{A} \prec_S \mathcal{A}$". ∎

While determining the preference relation between each pair of explanations is non-trivial, we present some properties for optimising the computation in certain special cases. The following result allows efficient checking of the preference relation and potentially pruning the search when explanations are obtained from (e.g., the instantiation of) other explanations.

Lemma 3. *For a QAP $\Lambda = (\mathcal{O}, \mathcal{D}, q, \Sigma)$ and a selection condition $S = (\Sigma_C, \Sigma_A, \Sigma_M)$, given two Σ-explanations $\mathcal{E}$ and $\mathcal{E}'$ to Λ, suppose there is a substitution σ such that $\mathcal{E}' = \mathcal{E}\sigma \setminus \mathcal{D}$, then*

- *$\mathcal{E} \preceq_S \mathcal{E}'$ iff $\mathcal{E}|_{\Sigma_C \cup \Sigma_M}\sigma = \mathcal{E}'|_{\Sigma_C \cup \Sigma_M}$ and $\sigma|_N$ is a renaming for the nulls $N = \mathsf{N}(\mathcal{E}|_{\Sigma_C})$; and*
- *$\mathcal{E}' \preceq_S \mathcal{E}$ iff there is a bipartition of the atoms in $\mathcal{E}'|_{\Sigma_A} = \mathcal{E}_1 \cup \mathcal{E}_2$ s.t. there exists a substitution σ' with $\mathcal{E}_1\sigma' \subseteq \mathcal{D}$ and $(\mathcal{E}_2 \cup \mathcal{E}'|_{\Sigma_M})\sigma' \subseteq \mathcal{E}$.*

Proof To show the "if" direction of the first statement, we want to show $\mathcal{E} \preceq_S \mathcal{E}'$. Let σ'' be a substitution such that $\sigma''|_{\mathsf{N}(\mathcal{E})} = \sigma|_{\mathsf{N}(\mathcal{E})}$ and $\sigma''|_N = \sigma|_N^-$ (note that $\sigma|_N$ is a renaming so its inverse is defined). We show that σ'' satisfies Conditions (i)–(iii) in the definition of $\preceq_S$. Since $\mathcal{E}|_{\Sigma_C \cup \Sigma_M}\sigma = \mathcal{E}'|_{\Sigma_C \cup \Sigma_M}$, $\mathcal{E}|_{\Sigma_C}\sigma = \mathcal{E}'|_{\Sigma_C}$. As σ is a renaming for N, $\mathcal{E}|_{\Sigma_C} = \mathcal{E}'|_{\Sigma_C}\sigma^-$, and $\mathcal{E}|_{\Sigma_C} =$

$\mathcal{E}'|_{\Sigma_C}\sigma''$; and Condition (i) is satisfied. Also, as $\mathcal{E}|_{\Sigma_M}\sigma = \mathcal{E}'|_{\Sigma_M}$, $\mathcal{E}|_{\Sigma_M}\sigma'' = \mathcal{E}'|_{\Sigma_M}$; and Condition (iii) is satisfied. Finally, as $\mathcal{E}' = \mathcal{E}\sigma\setminus\mathcal{D}$, $\mathcal{E}'|_{\Sigma_A} = \mathcal{E}|_{\Sigma_A}\sigma\setminus\mathcal{D}$, and $\mathcal{E}|_{\Sigma_A}\sigma \subseteq \mathcal{E}'|_{\Sigma_A} \cup \mathcal{D}$; and Condition (ii) is satisfied.

To show the "only if" direction of the first statement, we assume there is a substitution σ'' satisfying Conditions (i)–(iii) in the definition of $\preceq_S$, and we want to show σ satisfies the right-hand-side of the statement. From Condition (iii), $\mathcal{E}|_{\Sigma_M}\sigma'' \subseteq \mathcal{E}'|_{\Sigma_M}$, that is, $\mathcal{E}|_{\Sigma_M}\sigma'' \subseteq (\mathcal{E}\sigma\setminus\mathcal{D})|_{\Sigma_M}$. Thus, $\mathcal{E}|_{\Sigma_M}\sigma\cap\mathcal{D} = \emptyset$, as otherwise there are more than one atoms in $\mathcal{E}$ that can be unified and it contradicts to the representativeness and minimality of an explanation. Hence, $\mathcal{E}|_{\Sigma_M}\sigma = \mathcal{E}'|_{\Sigma_M}$. Also, from Condition (i), $\mathcal{E}|_{\Sigma_C} \subseteq \mathcal{E}'|_{\Sigma_C}\sigma''$, that is, $\mathcal{E}|_{\Sigma_C} \subseteq (\mathcal{E}\sigma\setminus\mathcal{D})|_{\Sigma_C}\sigma''$. Again, $\mathcal{E}|_{\Sigma_C}\sigma \cap \mathcal{D} = \emptyset$, as otherwise it contradicts to the representativeness and minimality of an explanation. Hence, $\mathcal{E}|_{\Sigma_C} = \mathcal{E}|_{\Sigma_C}\sigma\sigma''$, and σ must be a renaming on N. And $\mathcal{E}|_{\Sigma_C}\sigma = \mathcal{E}'|_{\Sigma_C}$, and $\mathcal{E}|_{\Sigma_C\cup\Sigma_M}\sigma = \mathcal{E}'|_{\Sigma_C\cup\Sigma_M}$.

To show the "if" direction of the second statement, we want to show $\mathcal{E}' \preceq_S \mathcal{E}$. Let σ'' be a substitution such that $\sigma''|_{\mathsf{N}(\mathcal{E})} = \sigma|_{\mathsf{N}(\mathcal{E})}$ and $\sigma''|_{\mathsf{N}(\mathcal{E}')} = \sigma'|_{\mathsf{N}(\mathcal{E}')}$. We show that σ'' satisfies Conditions (i)–(iii) in the definition of $\preceq_S$. As $\mathcal{E}' = \mathcal{E}\sigma\setminus\mathcal{D}$, $\mathcal{E}' \subseteq \mathcal{E}\sigma$ and $\mathcal{E}'|_{\Sigma_C} \subseteq \mathcal{E}|_{\Sigma_C}\sigma$; hence, $\mathcal{E}'|_{\Sigma_C} \subseteq \mathcal{E}|_{\Sigma_C}\sigma''$, and Condition (i) is satisfied. Also, as $\mathcal{E}'|_{\Sigma_A} = \mathcal{E}_1\cup\mathcal{E}_2$ s.t. there exists a substitution σ' with $\mathcal{E}_1\sigma' \subseteq \mathcal{D}$ and $(\mathcal{E}_2 \cup \mathcal{E}'|_{\Sigma_M})\sigma' \subseteq \mathcal{E}$, we have $\mathcal{E}'|_{\Sigma_A}\sigma' = \mathcal{E}_1\sigma' \cup \mathcal{E}_2\sigma' \subseteq \mathcal{D}|_{\Sigma_A} \cup \mathcal{E}|_{\Sigma_A}$. That is, $\mathcal{E}'|_{\Sigma_A}\sigma'' \subseteq \mathcal{D}\cup\mathcal{E}|_{\Sigma_A}$; and Condition (ii) is satisfied. Similarly, as $\mathcal{E}'|_{\Sigma_M}\sigma' \subseteq \mathcal{E}|_{\Sigma_M}$, $\mathcal{E}'|_{\Sigma_M}\sigma'' \subseteq \mathcal{E}|_{\Sigma_M}$; and Condition (iii) is satisfied.

To show the "only if" direction of the second statement, we assume there is a substitution σ'' satisfying Conditions (i)–(iii) in the definition of $\preceq_S$, and we want to show the right-hand-side of the statement. From Condition (ii), $\mathcal{E}'|_{\Sigma_A}\sigma'' \subseteq \mathcal{E}|_{\Sigma_A} \cup \mathcal{D}$, that is, $(\mathcal{E}\sigma \setminus \mathcal{D})|_{\Sigma_A}\sigma'' \subseteq \mathcal{E}|_{\Sigma_A} \cup \mathcal{D}$. Then, there is a bipartition $\mathcal{E}|_{\Sigma_A} = \mathcal{E}_1' \cup \mathcal{E}_2'$ such that $\mathcal{E}_1'\sigma\sigma'' \subseteq \mathcal{D}$ and $\mathcal{E}_2'\sigma\sigma'' \subseteq \mathcal{E}|_{\Sigma_A}$. Similarly, from Condition (iii), $\mathcal{E}'|_{\Sigma_M}\sigma'' \subseteq \mathcal{E}|_{\Sigma_M}$, that is, $(\mathcal{E}\sigma \setminus \mathcal{D})|_{\Sigma_M}\sigma'' \subseteq \mathcal{E}|_{\Sigma_M}$. Then, there is a bipartition $\mathcal{E}|_{\Sigma_M} = \mathcal{E}_1'' \cup \mathcal{E}_2''$ such that $\mathcal{E}_1''\sigma \subseteq \mathcal{D}$ and $\mathcal{E}_2''\sigma\sigma'' \subseteq \mathcal{E}|_{\Sigma_M}$; that is, $\mathcal{E}'|_{\Sigma_M} = \mathcal{E}_2''\sigma$. Let $\mathcal{E}_1 = \mathcal{E}_1'\sigma \setminus \mathcal{D}$, $\mathcal{E}_2 = (\mathcal{E}_2' \cup \mathcal{E}_2'')\sigma$, and $\sigma' = \sigma''$. Then, $\mathcal{E}_1\sigma' \subseteq \mathcal{D}$ and $(\mathcal{E}_2 \cup \mathcal{E}'|_{\Sigma_M})\sigma' \subseteq \mathcal{E}$. ∎

The lemma shows that when a Σ-explanation $\mathcal{E}'$ can be obtained from substituting nulls (and eliminating facts existing in $\mathcal{D}$ due to minimality) in another Σ-explanation $\mathcal{E}$, verifying $\mathcal{E} \preceq_S \mathcal{E}'$ (or $\mathcal{E}' \preceq_S \mathcal{E}$) requires only checking some relatively strict conditions on $\Sigma_C \cup \Sigma_M$ (resp., $\Sigma_A \cup \Sigma_M$). This is useful for the computation where explanations are incrementally generated.

The following properties are useful for the computation of selective explanations in some special cases. For two explanations $\mathcal{E}$ and $\mathcal{E}'$ such that $\mathcal{E}' = \mathcal{E}\sigma \setminus \mathcal{D}$ for some substitution σ, we say $\mathcal{E}$ is *at least as general as* $\mathcal{E}'$ and $\mathcal{E}'$ is *at least as specific as* $\mathcal{E}$. An explanation $\mathcal{E} \in \mathsf{exp}_\Sigma(\Lambda)$ is *most general* (or *most specific*) if for each explanation $\mathcal{E}' \in \mathsf{exp}_\Sigma(\Lambda)$, $\mathcal{E}'$ is at least as general (resp., specific) as $\mathcal{E}$ implies that $\mathcal{E}$ is also at least as general (resp., specific) as $\mathcal{E}'$. The following result is regarding the special cases where all abducibles are concrete, abstract, or mixed ones.

Proposition 1. *The following statements hold for a QAP Λ and a selection condition S,*

– *if* $S = (\Sigma, \emptyset, \emptyset)$ *then* $\mathsf{exp}_S(\Lambda)$ *contains only most specific ones in* $\mathsf{exp}_\Sigma(\Lambda)$*;*
– *if* $S = (\emptyset, \Sigma, \emptyset)$ *then* $\mathsf{exp}_S(\Lambda)$ *contains only most general ones in* $\mathsf{exp}_\Sigma(\Lambda)$*;*
– *if* $S = (\emptyset, \emptyset, \Sigma)$ *then* $\mathsf{exp}_S(\Lambda) = \mathsf{exp}_\Sigma(\Lambda)$*.*

Proof Consider the case where $S = (\Sigma, \emptyset, \emptyset)$, for each explanation $\mathcal{E} \in \mathsf{exp}_S(\Lambda)$, suppose there exists a Σ-explanation $\mathcal{E}'$ that is at least as specific as $\mathcal{E}$. We want to show that $\mathcal{E}$ is also at least as specific as $\mathcal{E}'$. From Lemma 3, $\mathcal{E}' \preceq_S \mathcal{E}$ trivially holds as $\mathcal{E}'|_{\Sigma_A \cup \Sigma_M} = \emptyset$. As $\mathcal{E} \in \mathsf{exp}_S(\Lambda)$, $\mathcal{E} \preceq_S \mathcal{E}'$ must hold. By Proposition 1, as $\Sigma = \Sigma_C$, $\mathcal{E}\sigma = \mathcal{E}'$ for a renaming σ. Hence, $\mathcal{E} = \mathcal{E}'\sigma^-$. As $\mathcal{E} \cap \mathcal{D} = \emptyset$, $\mathcal{E} = \mathcal{E}'\sigma^- \setminus \mathcal{D}$. That is, $\mathcal{E}$ is also at least as specific as $\mathcal{E}'$, and $\mathcal{E}$ is a most specific Σ-explanation.

Consider the case when $S = (\emptyset, \Sigma, \emptyset)$, for each explanation $\mathcal{E}' \in \mathsf{exp}_S(\Lambda)$, suppose there exists a Σ-explanation $\mathcal{E}$ that is at least as general as $\mathcal{E}'$. We want to show that $\mathcal{E}'$ is also at least as general as $\mathcal{E}$. From Lemma 3, $\mathcal{E} \preceq_S \mathcal{E}'$ trivially holds as $\mathcal{E}|_{\Sigma_C \cup \Sigma_M} = \mathcal{E}'|_{\Sigma_C \cup \Sigma_M} = \emptyset$. As $\mathcal{E}' \in \mathsf{exp}_S(\Lambda)$, $\mathcal{E}' \preceq_S \mathcal{E}$ must hold. By Proposition 1, as $\Sigma = \Sigma_A$, there is a bipartition $\mathcal{E}' = \mathcal{E}_1 \cup \mathcal{E}_2$ and a substitution σ such that $\mathcal{E}_1\sigma \subseteq \mathcal{D}$ and $\mathcal{E}_2\sigma \subseteq \mathcal{E}$. That is, $\mathcal{E}'\sigma \setminus \mathcal{D} \subseteq \mathcal{E}$. That is, $\mathcal{E}'$ is also at least as general as $\mathcal{E}$, and $\mathcal{E}'$ is a most general Σ-explanation.

Finally, when $S = (\emptyset, \emptyset, \Sigma)$, $\mathsf{exp}_S(\Lambda) = \mathsf{exp}_\Sigma(\Lambda)$ by definition. ∎

Intuitively, the proposition shows that when all the abducibles are concrete (or abstract) ones, the S-explanations are all most specific (resp., general) ones. Finally, the last statement in the proposition shows that the notion of S-explanations generalises the explanations in [12], which is the case when all the abducibles are mixed.

4 Rule Representation of Explanations

We have introduced a framework to allow users to select explanations based on their needs, and the selected collection of explanations can be much smaller compared to that of all the possible explanations. In this section, we propose a rule representation for explanations, which provides a simple and intuitive way for representing explanations using rules.

In the running example, each $\mathcal{E}_i = \{\mathit{high\_risk}(p_i)\}$ is an explanation because $\mathit{contact}(\mathit{Alice}, p_i)$ is a fact in the dataset $\mathcal{D}$. All the $\mathcal{E}_i$'s can be obtained from one general explanation $\mathcal{E}_v = \{\mathit{contact}(\mathit{Alice}, v), \mathit{high\_risk}(v)\}$; and if an instance of the form $\mathit{contact}(\mathit{Alice}, p)$ is found in $\mathcal{D}$ for some constant p then $\{\mathit{high\_risk}(p)\}$ is an explanation. Such a pattern can be captured by a rule $r : \mathit{high\_risk}(x) \Leftarrow \mathit{contact}(\mathit{Alice}, x)$, and all the explanations $\mathcal{E}_i$ can be derived by applying r to $\mathcal{D}$, and hence rule r can be seen as a compact representation for them. Note that the rule representations must not be confused with the rules in the ontology. It should be understood as if $\mathit{contact}(\mathit{Alice}, p)$ is found in the given dataset for some constant p then $\{\mathit{high\_risk}(p)\}$ is an explanation to the given observation.

To achieve this, we need to extend rules with negations in the bodies, that is, we consider rules r of the form

$$\forall\vec{x}.\forall\vec{y}.[\varphi(\vec{x},\vec{u}) \Leftarrow \psi(\vec{x},\vec{y}) \wedge \bigwedge_{i=1}^{n} \forall\vec{z}_i.\neg\psi_i(\vec{x},\vec{y},\vec{z}_i)],$$

where $\vec{x}$, $\vec{y}$ and $\vec{z}_i$ ($1 \le i \le n$) are pairwise disjoint vectors of variables, $\vec{u}$ is a vector of labelled nulls, and $\varphi(\vec{x},\vec{u})$, $\psi(\vec{x},\vec{y})$, and $\psi_i(\vec{x},\vec{y},\vec{z}_i)$ ($1 \le i \le n$) are conjunctions of atoms. The notions of $\mathsf{body}(r)$ and $\mathsf{head}(r)$ are also generalised. For a dataset $\mathcal{D}$, r is *applicable* to $\mathcal{D}$ if there is a substitution σ mapping all the variables in $\vec{x} \cup \vec{y}$ to constant such that $\mathcal{D} \models \mathsf{body}(r)\sigma$, and the result of applying r to $\mathcal{D}$ w.r.t. σ is $r(\mathcal{D},\sigma) = \mathsf{head}(r)\sigma$. $r(\mathcal{D})$ denotes the set of all the results of applying r to $\mathcal{D}$ with different substitution, and for a set of rules $\mathcal{R}$, $\mathcal{R}(\mathcal{D}) = \bigcup_{r\in\mathcal{R}} r(\mathcal{D})$.

Next, we define such rule representations for the explanations to a QAP. A rule r is *explanation-representing* (*exp-rep*) for a QAP Λ with a dataset $\mathcal{D}$ if each set of facts $\mathcal{A} \in r(\mathcal{D})$ is an explanation to Λ. In the above example, $\mathit{high\_risk}(x) \Leftarrow \mathit{contact}(\mathit{Alice}, x)$ is an exp-rep rule. Yet not all the explanations represented by such rules are necessarily minimal explanations. Even for a single rule r, it is possible that there exist two substitutions σ and σ' such that $r(\mathcal{D},\sigma)$ is a minimal explanation but $r(\mathcal{D},\sigma')$ is not.

Example 2. Consider a QAP with the dataset $\mathcal{D} = \{A(a,a), A(a,b), B(a)\}$ and abducibles $\Sigma = \{C, D\}$. Suppose two exp-rep rules are

$$r_1 : C(x,y,w) \wedge D(w) \Leftarrow A(x,y). \quad r_2 : C(x',x',v') \Leftarrow B(x').$$

Then, $r_1(\mathcal{D}) = \{\mathcal{E}_1, \mathcal{E}_2\}$ with $\mathcal{E}_1 = \{C(a,a,w), D(w)\}$ and $\mathcal{E}_2 = \{C(a,b,w), D(w)\}$, and $r_2(\mathcal{D}) = \{\mathcal{E}_3\}$ with $\mathcal{E}_3 = \{C(a,a,v')\}$. $\mathcal{E}_1$, $\mathcal{E}_2$ and $\mathcal{E}_3$ are all explanations, but $\mathcal{E}_1$ is not a minimal explanation, as $\mathcal{E}_3 \prec_m \mathcal{E}_1$, i.e., there exists renaming $\sigma = \{v'/w\}$ s.t. $\mathcal{E}_3\sigma \subset \mathcal{E}_1$. To capture only the minimal explanations, i.e., $\mathcal{E}_2$ but not $\mathcal{E}_1$, intuitively, r_1 need to be refined w.r.t. r_2 as follows

$$C(x,y,w) \wedge D(w) \Leftarrow A(x,y) \wedge \neg\big(x = y \wedge B(x)\big).$$

In what follows, we first define when a rule should be refined by another rule, so that the result of refinement can capture selective explanations. After that, we present the definition of the refinement.

Definition 2. *For a QAP with a dataset $\mathcal{D}$ and a selection condition S, a preference relation $\preceq \in \{\preceq_m, \preceq_h, \preceq_S\}$, two exp-rep rules r and r', and a substitution τ, we say r is* $\preceq$-refinable *by r' w.r.t. τ, denoted $r \ll_{\preceq,\tau} r'$, if for each substitution σ with which both $r\tau$ and $r'\tau$ are applicable to $\mathcal{D}$, $r'\tau(\mathcal{D},\sigma) \prec r\tau(\mathcal{D},\sigma)$.*

Intuitively, τ "unifies" $\mathsf{head}(r')$ and a subset of $\mathsf{head}(r)$ by unifying their variables and constants (while overlooking nulls), such that for *each* substitution σ with which both rules are applicable to $\mathcal{D}$, the explanation derived from $r'\tau$ is strictly preferred over that derived from $r\tau$. In Example 2, r_1 is $\preceq_m$-refinable by r_2 w.r.t. substitution $\tau = \{y/x, x'/x\}$, as for the substitution $\sigma = \{x/a\}$ which is the only one with which both $r_1\tau$ and $r_2\tau$ are applicable to $\mathcal{D}$, i.e., $\mathcal{D} \models (A(x,x) \wedge B(x))\sigma$, and $r_2\tau(\mathcal{D},\sigma) \prec_m r_1\tau(\mathcal{D},\sigma)$, i.e., $\{C(x,x,v')\}\sigma \prec_m \{C(x,x,w), D(w)\}\sigma$.

Note that each substitution τ defines an equivalence relation $\sim_\tau$ over $\mathsf{V} \cup \mathsf{C}$ such that for two terms t_1 and t_2, $t_1 \sim_\tau t_2$ iff $t_1\tau = t_2\tau$. For a term t, $[t]_\tau$ is the equivalence class for t under $\sim_\tau$, i.e., $[t]_\tau = \{t' \mid t \sim_\tau t'\}$. For a finite set of variables $X \subseteq \mathsf{V}$, w.l.o.g., we assume there is an order on the elements in X, i.e., $X = \{x_i \mid 1 \leq i \leq n\}$. Then, we define a formula that captures the equivalence relation on X introduced by τ, i.e.,

$$\begin{aligned}\varphi_\sim(X,\tau) = \bigwedge \big\{ x_i = x_j \mid 1 \leq i < j \leq n,\, x_j \in [x_i]_\tau,& \\ \text{and there is no } i < k < j \text{ s.t. } x_k \in [x_i]_\tau \big\} \wedge& \\ \bigwedge \big\{ x_i = a \mid 1 \leq i \leq n,\, a \in [x_i]_\tau \cap \mathsf{C},& \\ \text{and there is no } 1 \leq j < i \text{ s.t. } x_j \in [x_i]_\tau \big\}.&\end{aligned}$$

Also, we define a substitution where each variable is mapped to a variable from X in its equivalent class, i.e., $\gamma_\sim(X,\tau) = \{x/x_i \mid 1 \leq i \leq n,\, x \in [x_i]_\tau,\, x \neq x_i,$ and there is no $1 \leq j < i$ s.t. $x_j \in [x_i]_\tau\}$. For two substitutions τ and τ' , we say τ is *at least as general as* τ' if $\tau\sigma \subseteq \tau'$ for some substitution σ; and they are *equivalent* if they are both at least as general as each other.

Consider a QAP Λ with a selection condition S, a preference relation $\preceq \in \{\preceq_m, \preceq_h, \preceq_S\}$, and two exp-rep rules r, r'. A substitution τ is a *most general* substitution for the $\preceq$-refinement of r by r', if $r \ll_{\preceq,\tau} r'$ and for each substitution τ' with $r \ll_{\preceq,\tau'} r'$ that is at least as general as τ, τ is equivalent to τ'. Let $\Delta_\Lambda(r, r', \preceq)$ be a set consisting of one equivalent substitution for each most general substitution for the $\preceq$-refinement of r by r'. Then, $\Delta_\Lambda(r, r', \preceq)$ is always finite, as there are finitely many ways to map the variables in the bodies of r and r' to $\mathcal{D}$. Next, we define the refinement of exp-rep rules.

Definition 3. *For a QAP Λ, a selection condition S, a preference relation $\preceq \in \{\preceq_m, \preceq_h, \preceq_S\}$, and two exp-rep rules r, r', the* $\preceq$-refinement *of r by r' is the rule* $\mathsf{head}(r) \Leftarrow \mathsf{body}(r) \wedge \varphi_\Lambda(r, r', \preceq)$ *where*

$$\varphi_\Lambda(r, r', \preceq) = \bigwedge_{\tau \in \Delta_\Lambda(r,r',\preceq)} \forall \vec{z}. \neg\Big(\varphi_\sim(\mathsf{V}(r),\tau) \wedge \mathsf{body}(r')\gamma_\sim(\mathsf{V}(r),\tau)\Big),$$

and $\vec{z}$ consist of those variables in $\mathsf{body}(r')\gamma_\sim(\mathsf{V}(r),\tau)$ but not in r.

In Example 2, consider $\tau = \{y/x, x'/x\}$ and x, y, x' all belong to the same equivalence class. Let $X = \mathsf{V}(r_1) = \{x, y\}$, then $\varphi_\sim(X,\tau)$ is $x = y$ and $\gamma_\sim(X,\tau) = \{y/x, x'/x\}$. As τ is the only most general substitution (up to renaming) for the $\preceq_m$-refinement of r_1 by r_2, the refinement is $C(x,y,w) \wedge D(w) \Leftarrow A(x,y) \wedge \neg\big(x = y \wedge B(x)\big)$.

Proposition 2. *For a QAP Λ with a dataset $\mathcal{D}$, a selection condition S, a preference relation $\preceq \in \{\preceq_m, \preceq_h, \preceq_S\}$, and two exp-rep rules r, r', let r^* be the $\preceq$-refinement of r by r'. Then, (i) r^* is an exp-rep rule for Λ, and (ii) for each substitution σ, $r(\mathcal{D},\sigma) \notin r^*(\mathcal{D})$ iff there exists a substitution σ' satisfying $r'(\mathcal{D},\sigma') \prec r(\mathcal{D},\sigma)$.*

Proof To show the "if" direction of (ii), let τ and σ'' be two substitutions satisfying that $\tau\sigma''|_{\mathsf{V}(r)} = \sigma|_{\mathsf{V}(r)}$ and $\tau\sigma''|_{\mathsf{V}(r')} = \sigma'|_{\mathsf{V}(r')}$. Then, $\mathcal{D} \models (\mathsf{body}(r)\tau \wedge \mathsf{body}(r')\tau)\sigma''$ and $r'\tau(\mathcal{D},\sigma'') \prec r\tau(\mathcal{D},\sigma'')$. There must exist a most general substitution τ for the $\preceq$-refinement of r by r', i.e., $\tau \in \Delta_\Lambda(r, r', \preceq)$. As $\tau\sigma''|_{\mathsf{V}(r)} = \sigma|_{\mathsf{V}(r)}$, $[x]_\tau \subseteq [x]_\sigma$ for each $x \in \mathsf{V}(r)$. Hence, based on its definition, $\varphi_\sim(\mathsf{V}(r),\tau)\sigma$ is a tautology. To show $\mathcal{D} \models \exists\vec{z}.\mathsf{body}(r')\gamma_\sim(\mathsf{V}(r),\tau)\sigma|_{\mathsf{V}(r)}$, consider a bipartition $X \cup \vec{z}$ of the variables in $\mathsf{body}(r')\gamma_\sim(\mathsf{V}(r),\tau)$where $X \subseteq \mathsf{V}(r)$. From the definition of $\gamma_\sim(\mathsf{V}(r),\tau)$, for each variable $x \in X$, there is a variable $y \in \mathsf{V}(r')$ such that $x\tau = y\tau$. Hence $x\tau\sigma'' = y\tau\sigma''$, which is $x\sigma = y\sigma'$. Hence, take a substitution $\pi = \sigma'|_{\vec{z}}$, $\mathsf{body}(r')\gamma_\sim(\mathsf{V}(r),\tau)\sigma|_{\mathsf{V}(r)}\pi = \mathsf{body}(r')\sigma'$. As $\mathcal{D} \models \mathsf{body}(r')\sigma'$, $\mathcal{D} \models \exists\vec{z}.\mathsf{body}(r')\gamma_\sim(\mathsf{V}(r),\tau)\sigma|_{\mathsf{V}(r)}$. We have shown $\mathcal{D} \not\models \mathsf{body}(r^*)\sigma$.

To show the "only if" direction of (ii), $r(\mathcal{D},\sigma) \notin r^*(\mathcal{D})$ implies that $\mathcal{D} \models \mathsf{body}(r)\sigma$ and $\mathcal{D} \not\models \mathsf{body}(r^*)\sigma$. That is, $\mathcal{D} \models \exists\vec{z}.\big(\varphi_\sim(\mathsf{V}(r),\tau) \wedge \mathsf{body}(r')\gamma_\sim(\mathsf{V}(r),\tau)\big)\sigma$ for some substitution $\tau \in \Delta_\Lambda(r, r', \preceq)$. As $\mathcal{D} \models \varphi_\sim(\mathsf{V}(r),\tau)\sigma$, $[x]_\tau \subseteq [x]_\sigma$ for each $x \in \mathsf{V}(r)$. Hence, there exists a substitution σ'' satisfying $\tau\sigma''|_{\mathsf{V}(r)} = \sigma|_{\mathsf{V}(r)}$. As $\mathcal{D} \models \mathsf{body}(r)\sigma$, $\mathcal{D} \models \mathsf{body}(r)\tau\sigma''$. Also, since $\mathcal{D} \models \exists\vec{z}.\mathsf{body}(r')\gamma_\sim(\mathsf{V}(r),\tau)\sigma$, there exists a substitution π with $\mathcal{D} \models \mathsf{body}(r')\gamma_\sim(\mathsf{V}(r),\tau)\sigma\pi$. Let $\tau\sigma''|_{\vec{z}} = \sigma\pi|_{\vec{z}}$. Then, $\mathcal{D} \models \mathsf{body}(r')\tau\sigma''$. That is, $\mathcal{D} \models (\mathsf{body}(r)\tau \wedge \mathsf{body}(r')\tau)\sigma''$. By the definition of $\Delta_\Lambda(r, r', \preceq)$, $r'\tau(\mathcal{D},\sigma'') \prec r\tau(\mathcal{D},\sigma'')$, which is $r'(\mathcal{D},\tau\sigma'') \prec r(\mathcal{D},\sigma)$. Then, let $\sigma'|_{\mathsf{V}(r')} = \tau\sigma''|_{\mathsf{V}(r')}$, we have $r'(\mathcal{D},\sigma') \prec r(\mathcal{D},\sigma)$. ∎

5 Computing Explanations and Rule Representations

In this section, we introduce methods for computing selective explanations and their rule representations for first-order rewritable QAPs. Given a QAP with an observation q and an ontology $\mathcal{O}$, q is *first-order rewritable* or simply *rewritable* w.r.t. $\mathcal{O}$ if there exists a finite set of BCQs, denoted as $\mathsf{rew}(q,\mathcal{O})$, such that for each dataset $\mathcal{D}$, $\mathcal{O} \cup \mathcal{D} \models q$ if and only if $\mathcal{D} \models q'$ for some BCQ $q' \in \mathsf{rew}(q,\mathcal{O})$. For simplicity, we also call such a QAP *rewritable*. First-order rewritability w.r.t. existential rules and efficient rewriting systems have been well studied [1, 14, 15]. We assume $\mathsf{rew}(q,\mathcal{O})$ is non-redundant, that is, there do not exist two BCQs $q_1, q_2 \in \mathsf{rew}(q,\mathcal{O})$ such that $q_1 \prec_h q_2$. We call each $q' \in \mathsf{rew}(q,\mathcal{O})$ a *rewriting* of q. For the convenience of discussion, we may equal a BCQ q with the set of atoms in it, and we assume a fixed bijective mapping $\rho : \mathsf{V} \to \mathsf{N}$, which allows us to map a BCQ to a QAP explanation.

We present a connection between S-explanations and rewriting. To achieve this, we consider facts in the dataset as rules with empty bodies. For a dataset $\mathcal{D}$, $\mathcal{R}_\mathcal{D}$ denotes the set of rules $\{P(\vec{a}) \leftarrow\ \mid P(\vec{a}) \in \mathcal{D}\}$. Given a set $\mathcal{Q}$ of BCQs and a signature Σ, $\mathcal{Q}|_\Sigma = \{q \in \mathcal{Q} \mid \mathsf{sig}(q) \subseteq \Sigma\}$. For a set of explanations Ξ to a QAP and a selection condition S, $\min_{\preceq_S}(\varXi)$ consists of all the explanations $\mathcal{E} \in \varXi$ such that for each explanation $\mathcal{E}' \in \varXi$ with $\mathcal{E}' \preceq_S \mathcal{E}$, $\mathcal{E} \preceq_S \mathcal{E}'$.

Proposition 3. *For a rewritable QAP $\varLambda = (\mathcal{O}, \mathcal{D}, q, \varSigma)$ and a selection condition S, $\mathsf{exp}_S(\varLambda) \equiv \min_{\preceq_S}\big(\mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})|_{\varSigma}\rho\big)$.*

Proof We only need to show that $\mathsf{exp}_{\varSigma}(\varLambda) \equiv \mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})|_{\varSigma}\rho$.

($\Rightarrow$) We want to show for each $\mathcal{E} \in \mathsf{exp}_{\varSigma}(\varLambda)$, there exists a BCQ $q' \in \mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$ over $\varSigma$ s.t. $\mathcal{E} \equiv q'\rho$. By the definition of a $\varSigma$-explanation, $\mathcal{O} \cup \mathcal{R}_{\mathcal{D}} \cup \mathcal{E} \models q$. By the definition of rewriting, there exists a BCQ $q' \in \mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$ s.t $\mathcal{E} \models q'$. Thus, $q'\rho \preceq_h \mathcal{E}$. Also, as $\mathsf{sig}(\mathcal{E}) \subseteq \varSigma$, $\mathsf{sig}(q') \subseteq \varSigma$. Moreover, as $q'\rho \models q'$, by the definition of rewriting, $\mathcal{O} \cup \mathcal{R}_{\mathcal{D}} \cup q'\rho \models q$. Hence, $q'\rho$ is an explanation to $\varLambda$. As $\mathcal{E} \in \mathsf{exp}_{\varSigma}(\varLambda)$, $\mathcal{E} \preceq_h q'\rho$ must hold. That is, $\mathcal{E} \equiv q'\rho$.

($\Leftarrow$) We want to show for each BCQ $q' \in \mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$ over $\varSigma$, there exists a $\varSigma$-explanation $\mathcal{E} \in \mathsf{exp}_{\varSigma}(\varLambda)$ s.t. $q'\rho \equiv \mathcal{E}$. As $q'\rho \models q'$, by the definition of rewriting, $\mathcal{O} \cup \mathcal{R}_{\mathcal{D}} \cup q'\rho \models q$. Hence, $q'\rho$ is an explanation to $\varLambda$. Assume $q'\rho$ is not equivalent to any $\varSigma$-explanation in $\mathsf{exp}_{\varSigma}(\varLambda)$, then there must exist a $\varSigma$-explanation $\mathcal{E}' \in \mathsf{exp}_{\varSigma}(\varLambda)$ s.t. $\mathcal{E}' \prec_h q'\rho$. From the above discussion, there exists a BCQ $q'' \in \mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$ with $\mathcal{E}' \equiv q''\rho$. Hence, $q''\rho \prec_h q'\rho$, and that is, $q'' \prec_h q'$, which contradicts to the non-redundant assumption of $\mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$. Hence, $q'\rho$ must be equivalent to some $\varSigma$-explanation $\mathcal{E} \in \mathsf{exp}_{\varSigma}(\varLambda)$. ∎

The result shows that the computation of S-explanations can utilise an efficient query rewriting system, which can potentially scale over large datasets.

Next, we consider some special cases where the computation can potentially be significantly simplified. For a BCQ q, an ontology $\mathcal{O}$ and a dataset $\mathcal{D}$, $\mathsf{rew}^*(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$ consists of all the BCQs $q' \in \mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$ such that q' cannot be rewritten by any rule in $\mathcal{R}_{\mathcal{D}}$. Given a signature $\varSigma$, $\mathsf{rew}^{\dagger}_{\varSigma}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$ consists of all the BCQs $q' \in \mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$ such that $\mathsf{sig}(q') \subseteq \varSigma$ and there exists no BCQ $q'' \in \mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$ with $\mathsf{sig}(q'') \subseteq \varSigma$ from which q' can be obtained by rewriting with rules in $\mathcal{R}_{\mathcal{D}}$. For example, consider $q = \{A(x,y)\}$, $\mathcal{O} = \{A(x,y) \leftarrow B(x,y), C(y,z), D(z)\}$, $\mathcal{D} = \{B(a,b), C(b,c)\}$, and $\varSigma = \{C, D\}$. Then, we have $\mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}}) = \{q_1, q_2, q_3, q_4, q_5\}$ with $q_1 = \{A(x,y)\}$, $q_2 = \{B(x,y), C(y,z), D(z)\}$, $q_3 = \{C(b,z), D(z)\}$, and $q_4 = \{D(c)\}$, whereas $\mathsf{rew}^*(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}}) = \{q_1, q_4\}$ and $\mathsf{rew}^{\dagger}_{\varSigma}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}}) = \{q_3\}$.

Proposition 4. *For a rewritable QAP $\varLambda = (\mathcal{O}, \mathcal{D}, q, \varSigma)$ and a selection condition S,*

- *if $S = (\varSigma, \emptyset, \emptyset)$, $\mathsf{exp}_S(\varLambda) \equiv \min_{\preceq_S}\big(\mathsf{rew}^*(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})|_{\varSigma}\rho\big)$;*
- *if $S = (\emptyset, \varSigma, \emptyset)$, $\mathsf{exp}_S(\varLambda) \equiv \mathsf{rew}^{\dagger}_{\varSigma}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})\rho$.*
- *if $S = (\emptyset, \emptyset, \varSigma)$, $\mathsf{exp}_S(\varLambda) \equiv \mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})|_{\varSigma}\rho$;*

Proof For the case when $S = (\varSigma, \emptyset, \emptyset)$, as $\mathsf{rew}^*(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}}) \subseteq \mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$, by Proposition 3, for each BCQ $q' \in \mathsf{rew}^*(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$ with $q'\rho \in \min_{\preceq_S}\big(\mathsf{rew}^*(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})|_{\varSigma}\rho\big)$, $q'\rho$ is equivalent to some explanation in $\mathsf{exp}_S(\varLambda)$. Conversely, for each explanation $\mathcal{E} \in \mathsf{exp}_S(\varLambda)$, by Proposition 3, there exists a BCQ $q' \in \mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$ with $q'\rho \in \min_{\preceq_S}\big(\mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})|_{\varSigma}\rho\big)$ s.t. $q'\rho$ is equivalent to $\mathcal{E}$.

We want to show $q' \in \mathsf{rew}^*(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$. Suppose otherwise, $q' \notin \mathsf{rew}^*(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$. Then, q' can be rewritten by a rule in $\mathcal{R}_{\mathcal{D}}$ into q''. Thus, there exists a substitution σ s.t. $q'\rho\sigma \cap \mathcal{D} \neq \emptyset$ and $q''\rho = q'\rho\sigma \setminus \mathcal{D}$. That is, $q''\rho$ is strictly more specific than $q'\rho$. Also, as $q''\rho \in \mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})|_{\Sigma}\rho$, by the proof of Proposition 3, $q''\rho$ is a Σ-explanation, and it contradicts to the first statement in Proposition 1. Hence, $q' \in \mathsf{rew}^*(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$.

For the case when $S = (\emptyset, \Sigma, \emptyset)$, we first show $\mathsf{exp}_S(\Lambda) \equiv \min_{\preceq_S} \big(\mathsf{rew}^{\dagger}_{\Sigma}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})\rho\big)$. Similar as above, for each BCQ $q' \in \mathsf{rew}^{\dagger}_{\Sigma}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$, $q'\rho$ is equivalent to some explanation in $\mathsf{exp}_S(\Lambda)$. Conversely, for each explanation $\mathcal{E} \in \mathsf{exp}_S(\Lambda)$, there exists a BCQ q' with $q'\rho \in \mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})|_{\Sigma}\rho$ s.t. $q'\rho$ is equivalent to $\mathcal{E}$. We want to show $q' \in \mathsf{rew}^{\dagger}_{\Sigma}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$. Suppose otherwise, $q' \notin \mathsf{rew}^{\dagger}_{\Sigma}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$. As $\mathsf{sig}(q') \subseteq \Sigma$. Then, q' can be obtained by rewriting a BCQ $q'' \in \mathsf{rew}^{\dagger}_{\Sigma}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$ by rules in $\mathcal{R}_{\mathcal{D}}$. Thus, $q''\rho$ is strictly more general than $q'\rho$ and $q''\rho$ is a Σ-explanation, and it contradicts to the second statement in Proposition 1. Hence, $q' \in \mathsf{rew}^{\dagger}_{\Sigma}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$.

Next, we show that $\min_{\preceq_S} \big(\mathsf{rew}^{\dagger}_{\Sigma}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})\rho\big) = \mathsf{rew}^{\dagger}_{\Sigma}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})\rho$. Towards a contradiction, suppose there are two BCQs $q_1, q_2 \in \mathsf{rew}^{\dagger}_{\Sigma}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$ with $q_1\rho \preceq_S q_2\rho$, that is, $q_1\sigma \subseteq q_2 \cup \mathcal{D}$ for some substitution σ. Suppose $q_1\sigma \subseteq q_2$, then $q_1 \preceq_h q_2$, which contradicts the non-redundancy of $\mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$. Otherwise, $q_1\sigma \cap \mathcal{D} \neq \emptyset$, then a BCQ $q_1' = q_1\sigma \setminus \mathcal{D}$ can be obtained by rewriting q_1 with rules in $\mathcal{R}_{\mathcal{D}}$, and $q_1' \preceq_h q_2$. Again, it contradicts the non-redundancy of $\mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$.

Finally, the third statement directly follows Proposition 1 and the proof of Proposition 3. ∎

The first statement of the proposition says when all the abducibles are concrete ones, the S-explanations can be generated with a greedy approach in instantiation, i.e., when it comes to rewriting by rules in $\mathcal{R}_{\mathcal{D}}$, the rules are applied in an exhaustive manner. The second statement shows when all the abducibles are abstract ones, instantiation via the rules in $\mathcal{R}_{\mathcal{D}}$ can be avoided as much as possible. Since in practice, the sizes of the datasets are often significantly larger than those of $\mathsf{rew}(q, \mathcal{O} \cup \mathcal{R}_{\mathcal{D}})$, the number of S-explanations in this case can be significantly smaller than that of Σ-explanations.

In what follows, we introduce the computation of rule representations. Note that the rewriting process can be done in two steps, by first rewriting with rules in $\mathcal{O}$ and then instantiating the rewritings with rules in $\mathcal{R}_{\mathcal{D}}$. Based on the intuition of rule representations, $\mathsf{rew}(q, \mathcal{O})$ can be a starting point to construct exp-rep rules. In particular, for a BCQ $q' \in \mathsf{rew}(q, \mathcal{O})$, an explanation to the QAP may be obtained from a bipartition of it $q' = q'_D \cup q'_E$, where $q'_D\sigma \subseteq \mathcal{D}$ for some substitution σ, $q'_E\sigma \cap \mathcal{D} = \emptyset$ and $\mathsf{sig}(q'_E) \subseteq \Sigma$, and $q'_E\sigma$ would form an explanation. We call such a bipartition of a rewriting *explanation-forming* (*exp-form*) for Λ. A rule can be constructed from it, $r_{(q'_E, q'_D)} : \varphi_E \Leftarrow \varphi_D$, where φ_E and φ_D are conjunctions of the atoms in respectively q'_E and q'_D and each variable in $\mathsf{V}(q'_E) \setminus \mathsf{V}(q'_D)$ is replaced with a distinct null.

For a rewritable QAP Λ, let $\mathcal{R}_{\Lambda}$ consists of all the rules $r_{(q_E, q_D)}$ where (q_E, q_D) is an exp-form bipartition for Λ, and $\mathsf{sol}(\Lambda)$ is the set of explanations to $\mathit{\Lambda}$. The following result shows that the set of rules constructed from exp-form bipartition of writings can capture the Σ-explanations of the QAP.

Lemma 4. *For a rewritable QAP $\mathit{\Lambda}$ with a dataset $\mathcal{D}$, $\mathsf{exp}_{\Sigma}(\mathit{\Lambda}) \subseteq \mathcal{R}_{\mathit{\Lambda}}(\mathcal{D}) \subseteq \mathsf{sol}(\mathit{\Lambda})$.*

Proof We first show for each explanation $\mathcal{E} \in \mathsf{exp}_{\Sigma}(\mathit{\Lambda})$ is in $\mathcal{R}_{\mathit{\Lambda}}(\mathcal{D})$. We have $\mathsf{sig}(\mathcal{E}) \subseteq \Sigma$ and $\mathcal{O} \cup \mathcal{D} \cup \mathcal{E} \models q$. By the definition of rewriting, there exists a BCQ $q' \in \mathsf{rew}(q, \mathcal{O})$ satisfying $\mathcal{E} \cup \mathcal{D} \models q'$. That is, there exists a substitution σ s.t. $q'\sigma \subseteq \mathcal{E} \cup \mathcal{D}$. Let q'_E and q'_D denote the set of atoms mapped to respectively $\mathcal{E}$ and $\mathcal{D}$ by σ. From the minimality of a Σ-explanation, $q'_E\sigma = \mathcal{E}$ and $q'_E\sigma \cap \mathcal{D} = \emptyset$. By the definition, $r_{(q'_E, q'_D)}$ is an exp-rep rule and $r_{(q'_E, q'_D)}(\mathcal{D}, \sigma) = \mathcal{E}$. That is, $\mathcal{E} \in \mathcal{R}_{\mathit{\Lambda}}(\mathcal{D})$.

Next, we show each set of facts $\mathcal{E} \in \mathcal{R}_{\mathit{\Lambda}}(\mathcal{D})$ is a Σ-explanation to $\mathit{\Lambda}$. By the definition, there exists a BCQ $q' \in \mathsf{rew}(q, \mathcal{O})$, a bipartition $q' = q'_D \cup q'_E$, and a substitution σ satisfying $r_{(q'_E, q'_D)}(\mathcal{D}, \sigma) = \mathcal{E}$ and $\mathsf{sig}(q'_E) \subseteq \Sigma$, that is, $\mathsf{sig}(\mathcal{E}) \subseteq \Sigma$. Also, as $\mathcal{E} \cup \mathcal{D} \models q'$, by the definition of rewriting, $\mathcal{O} \cup \mathcal{D} \cup \mathcal{E} \models q$. Hence, $\mathcal{E}$ is a Σ-explanation to $\mathit{\Lambda}$. ∎

For a set of exp-rep rules $\mathcal{R}$ and a preference relation $\preceq \in \{\preceq_m, \preceq_h, \preceq_S\}$, the *$\preceq$-refinement* of $\mathcal{R}$ w.r.t. $\mathit{\Lambda}$ is $\mathsf{ref}_{\preceq}(\mathcal{R}) = \{\mathsf{head}(r) \Leftarrow \mathsf{body}(r) \wedge \bigwedge_{r' \in \mathcal{R}_{\mathit{\Lambda}}} \varphi_{\mathit{\Lambda}}(r, r', \preceq) \mid r \in \mathcal{R}\}$, where $\varphi_{\mathit{\Lambda}}(r, r', \preceq)$ is defined as in Definition 3. The following result shows the set of S-explanations can be captured by a set of exp-rep rules obtained through refinement.

Proposition 5. *For a rewritable QAP $\mathit{\Lambda}$ with a dataset $\mathcal{E}$ and a selection condition S, let $\mathcal{R}^*_{\mathit{\Lambda}} = \mathsf{ref}_{\preceq_S}\Big(\mathsf{ref}_{\preceq_h}\big(\mathsf{ref}_{\preceq_m}(\mathcal{R}_{\mathit{\Lambda}})\big)\Big)$. Then, $\mathsf{exp}_S(\mathit{\Lambda}) \equiv \mathcal{R}^*_{\mathit{\Lambda}}(\mathcal{D})$.*

Proof ($\Rightarrow$) We want to show for each explanation $\mathcal{E} \in \mathsf{exp}_S(\mathit{\Lambda})$, $\mathcal{E} \in \mathcal{R}^*_{\mathit{\Lambda}}(\mathcal{D})$. By Lemma 4, $\mathcal{E} \in \mathcal{R}_{\mathit{\Lambda}}(\mathcal{D})$. There exists an exp-rep rule $r \in \mathcal{R}_{\mathit{\Lambda}}$ and a substitution σ s.t. $r(\mathcal{D}, \sigma) = \mathcal{E}$. If $\mathcal{E} \notin \mathcal{R}^*_{\mathit{\Lambda}}(\mathcal{D})$, then there must be an exp-rep rule $r' \in \mathcal{R}_{\mathit{\Lambda}}$ s.t. r is $\preceq$-refinable by r' with some substitution $\tau \in \Delta_{\mathit{\Lambda}}(r, r', \preceq)$, where $\preceq \in \{\preceq_m, \preceq_h, \preceq_S\}$. Then, there exists a substitution σ' s.t. $\sigma = \tau\sigma'$, and $r'(\mathcal{D}, \tau\sigma') \prec r(\mathcal{D}, \tau\sigma') = \mathcal{E}$. Again, by Lemma 4, $r'(\mathcal{D}, \tau\sigma')$ is a Σ-explanation to $\mathit{\Lambda}$. It contradicts to the fact $\mathcal{E} \in \mathsf{exp}_S(\mathit{\Lambda})$. Hence, $\mathcal{E} \in \mathcal{R}_{\mathit{\Lambda}}(\mathcal{D})$.

($\Leftarrow$) We want to show for each set of facts $\mathcal{E} \in \mathcal{R}^*_{\mathit{\Lambda}}(\mathcal{D})$, $\mathcal{E} \in \mathsf{exp}_S(\mathit{\Lambda})$. There exists an exp-rep rule $r \in \mathcal{R}^*_{\mathit{\Lambda}}$ and a substitution σ s.t. $r(\mathcal{D}, \sigma) = \mathcal{E}$. By Lemma 4, $\mathcal{E} \in \mathsf{sol}(\mathcal{D})$. If $\mathcal{E} \notin \mathsf{exp}_S(\mathit{\Lambda})$, then there must be an explanation $\mathcal{E}' \in \mathsf{exp}_{\Sigma}(\mathit{\Lambda})$ s.t. $\mathcal{E}' \prec \mathcal{E}$ for $\preceq \in \{\preceq_m, \preceq_h, \preceq_S\}$. Again, by Lemma 4, $\mathcal{E}' \in \mathcal{R}_{\mathit{\Lambda}}(\mathcal{D})$ and there exists an exp-rep rule $r' \in \mathcal{R}_{\mathit{\Lambda}}$ and a substitution σ' s.t. $r'(\mathcal{D}, \sigma') = \mathcal{E}'$. Then, r is $\preceq$-refinable by r' with some substitution $\tau \in \Delta_{\mathit{\Lambda}}(r, r', \preceq)$, which contradicts to the fact $\mathcal{E} \in \mathcal{R}^*_{\mathit{\Lambda}}(\mathcal{D})$. ∎

6 Experiments

We have implemented a prototype system for the computation of selective explanations based on Drewer [21], a rewriting-based query answering system for existential rules. We have conducted two sets of experiments to evaluate the scalability of our system and the sizes of various types of explanations.

– In the first set of experiments, we used standard benchmarks and compared our system with similar QAP systems, which demonstrates the superior time efficiency and compactness of our system. It shows our system is scalable over large-scale datasets and complex observations, and the sizes of our explanations are quite manageable for most cases, especially for abstract explanations and rule representations.
– In the second set of experiments, we further analyse the scalability of our system using a configurable real-life benchmark from natural language question answering. We also demonstrate the potential usefulness of our explanations with some samples.

All experiments were performed on a server with Intel Xeon CPU at 2.70GHz CPU and 16GB of RAM, with the maximum Java heap size set to 8GB.

6.1 Standard OQA Benchmarks

For the first set of experiments, we adopted several commonly used benchmarks for ontology-mediated query answering, including three ontologies in description logics, LSTW, Semintec and Vicodi, as well as two with more expressive existential rules (with predicates of arities more than two) [3], STB-128 and ONT-256. The numbers of rules in these ontologies range from 197 to 529, and the numbers of facts in their accompanying datasets range from 65K to 2M.

For each ontology, we used 5 BCQs as observations. Each BCQ is obtained from an existing CQ from the benchmark by removing the answer variables and replacing some other variables with constants. It guarantees that none of the BCQs is entailed by the ontologies (together with their datasets), so that the QAP is non-trivial in a sense that no explanation should be empty. The difficulty of a QAP largely depends on the number of variables in the observation. For the first three benchmarks, in order to compare with a baseline ABEL [22], we used BCQs without variables. For the other two benchmarks, unlike many evaluations using observations with at most one variable, we challenge our systems with observations with up to 21 variables each. For each ontology and each BCQ observation, all the predicates in the ontology are specified as the abducibles.

For existing systems on QAP, neither ABEL nor the system in [12] can handle all the benchmarks we evaluated. We have included the results of ABEL on the benchmarks it can handle. For the system in [12], as their explanations are a special case for S-explanations, we use our system to generate them (Mixed). For each QAP evaluated, we compare the sizes of explanations and the times used for generating them. Besides Mixed, we consider two special cases where all abducibles are abstract (Abstract) and all of them are concrete (Concrete). The sizes of explanations are measured by the total numbers of atoms in all the explanations, when the explanations are expressed as facts (F) and rules (R).

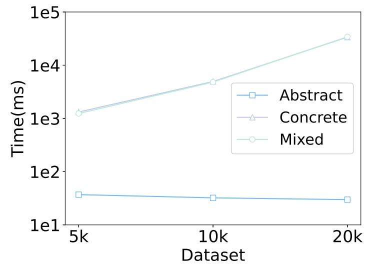
For Abstract, the sizes of facts and rules are the same[4]. The results are shown in Table 1, and all times are in milliseconds.

Table 1. Evaluation on standard OQA benchmarks.

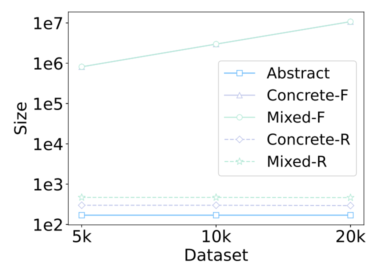
Ontology	Query	Abstract		Concrete			Mixed			ABEL	
		F/R	Time	R	F	Time	R	F	Time	F	Time
LSTW	q1	4	3	4	4	6	4	4	6	12	287
	q2	2	185	2	2	167	2	2	161	3	1K
	q3	46	26	46	46	69	46	46	47	150	974
	q4	168	147	168	168	251	168	168	185	889	505K
	q5	4	142	4	4	90	4	4	93	6	155K
Semintec	q1	2	11	2	2	13	2	2	12	27	651K
	q2	22	44	22	22	54	22	22	48	109	14K
	q3	16	13	16	16	28	16	16	31	72	6K
	q4	60	56	60	60	79	60	60	84	72	6K
	q5	18	6	18	18	15	18	18	19	150	27K
Vicodi	q1	3	3	3	3	4	3	3	3	9	310
	q2	250	226	250	250	379	250	250	353	810	175K
	q3	48	21	48	48	45	48	48	34	144	14K
	q4	40	29	40	40	51	40	40	48	100	7K
	q5	74	32	74	74	62	74	74	54	222	38K
STB-128	q1	72	11	1	47	4K	73	119	5K	-	-
	q2	12	4	6	29K	1K	15	29K	1K	-	-
	q3	24	3	2	146	1K	26	170	1K	-	-
	q4	200	59	73	440K	8K	208	440K	7K	-	-
	q5	576	141	160	1M	6K	736	1M	6K	-	-
ONT-256	q1	96	25	1	18	6K	97	114	6K	-	-
	q2	1K	464	704	4M	14K	1K	4M	13K	-	-
	q3	96	8	19	89K	5K	103	89K	5K	-	-
	q4	60	9	2	94	4K	62	154	4K	-	-
	q5	120	7	72	310K	2K	152	310K	2K	-	-

We can see that when explanations are expressed as facts, the sizes of Abstract explanations are significantly smaller than Concrete and Mixed ones. Hence, when retrieving specific individuals is not strictly necessary, abstract explanations are preferred for computational efficiency and brevity. Concrete and Mixed explanations expressed as facts are often several magnitudes larger than their counterparts in the form of rules, which indicates most explanations share similar patterns. Hence, when retrieving individuals are necessary, representing the explanations as rules may significantly enhance their brevity. Also, while computing Concrete explanations may take more time than for Mixed ones due to more complex preference checking, the explanation sizes can sometimes be significantly smaller than Mixed ones (e.g., q1 for ONT-256). ABEL computes

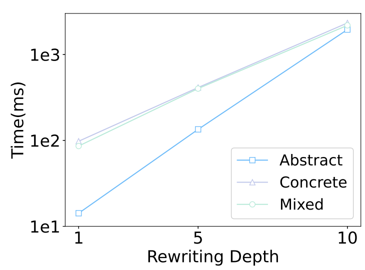
[4] From Propositions 4 and 5, when the abducibles include all the predicates, the explanations as facts and as rules are both those in $\mathsf{rew}(q, \mathcal{O})$.



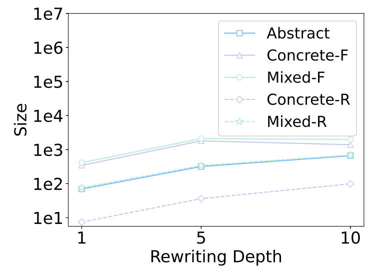
(a) Times with varying data sizes.



(b) Exp. sizes with varying data sizes.



(c) Times with varying depths.



(d) Exp. sizes with varying depths.

Fig. 1. Evaluation on the NLP question answering benchmark.

explanations according to a different definition where the use of nulls is not permitted. We can see that for simple observations without variables, ABEL took significantly more time and the sizes of explanations are much larger compared to ours.

6.2 NLP Question Answering Benchmark

In our second set of experiments, we used the benchmark in [18] based on natural language questions over DBpedia [16]. This benchmark shows the potential of our explanations in real-life applications such as question answering, and it also allows us to configure the complexity of the ontology and the size of the dataset.

The observations are generated from questions in LC-Quad [20], and for each setting, we used 5 observations with 2 or 3 atoms each. We evaluate computation times and explanation sizes over data sizes ranging from 5K, 10K to 20K, and various rewriting depths (depth being 1, 5, or 10). The numbers of applicable rule (in rewriting) are kept between 38 – 363. The results are shown in Figure 1, averaged over the 5 observations.

It can be seen that for Concrete and Mixed, the computation times and explanation sizes increase moderately as the data size increases, as expected, whereas Abstract and rule representations are not affected by data sizes. On the other hand, the computation times and explanation sizes for all the three types of explanations are sensitive to the increase of rewriting depth, which is due to the connection between explanation and rewriting.

We also conducted a qualitative analysis on our explanations over NLP question answering. Table 2 shows some observations in English (Q), their SPARQL equivalent (q), ontological rules applicable (r), known facts in DBpedia (f), and our explanations both as facts $\mathcal{E}$ and in English (E) obtained through a manual translation.

Table 2. Sample explanations on NLP question answering.

Q	*Is Tea the main ingredient of Lahpet?*
q	ASK WHERE { dbr:Lahpet dbp:mainIngredient dbr:Tea }
r	dbp:mainIngredient$(X, Y) \leftarrow$ dbp:similarDish$(Z, X) \wedge$ dbo:ingredient(Z, Y)
f	dbo:Ingredient(dbr:Butter_tea, dbr:Tea)
$\mathcal{E}$	dbp:similarDish(dbr:Butter_tea, dbr:Laphet)
E	*Butter tea and Lahpet are similar dishes.*
Q	*Is Tea the main ingredient of Lahpet?*
q	ASK WHERE { dbr:Lahpet dbp:mainIngredient dbr:Tea }
r	dbp:mainIngredient$(X, Y) \leftarrow$ dbo:hasVariant$(Z, X) \wedge$ dbo:ingredient(Z, Y)
f	none
$\mathcal{E}$	dbo:hasVariant(X, dbr:Laphet), dbo:ingredient(X, dbr:Tea)
E	*The ingredient of some variant of Lahpet is Tea.*
Q	*Was Kevin Jonas a part of Jonas Brothers?*
q	ASK WHERE { dbr:Jonas_Brothers dbo:formerBandMember dbr:Kevin_Jonas }
r	dbo:formerBandMember$(X, Y) \leftarrow$ dbo:associatedBand(Y, X)
f	none
$\mathcal{E}$	dbo:associatedBand(dbr:Danielle_Jonas, dbr:Jonas_Brothers)
E	*The associated band of Kevin Jonas is Jonas Brothers.*

7 Related Work

Equipping ontology-mediated query answering systems with explanation facilities has drawn significant interests in recent years. Early work mainly focuses on *axiom pinpointing* [19] in description logics, in which explanations are minimal subsets of the ontologies that entails a given subsumption. These explanations are often called *justifications*. While the problem of explaining query answers for CQs is first considered in [5] for DL-Lite ontologies, unlike the query abduction problem, explanations for query answers are minimal subsets of the datasets that support the answers. In [4], the authors consider explaining query answers for DL-Lite, in the context of consistent query answering, i.e., the dataset is inconsistent with the ontology. In [10, 11], the authors study the problem in various settings for a range of description logics and existential rules. Apart from the traditional settings, they also propose to find explanations that include or exclude a given set of facts.

Query abduction is also known as explaining *negative answers*, which is first formally defined by [9]. The authors focused on the complexity of query abduction in DL-Lite. In [12], the authors consider the preference between QAP explanations and present a method for computing the explanations through query rewriting. As we discussed before, the generated explanations are a mix of high level (abstract) and low level (concrete) explanations. This work was then extended to possibly inconsistent ontologies, by adapting inconsistency-tolerant querying semantics [13]. In [22], the authors present a scalable query abduction approach for $\mathcal{EL}$ ontologies, yet it does not allow nulls in the explanations. All these approaches define an explanation as a set of facts, whereas we introduce a rule representation of explanations.

8 Conclusion

In this paper, we propose a novel notion of selective explanations, which allows the user to characterise and distinguish abstract and concrete explanations. From a theoretical perspective, it generalises the existing notion of explanations for query abduction problems; and from a practical point of view, the numbers of selective explanations can be significantly smaller than those of total explanations. To further reduce the numbers and enhance the brevity of the explanations, we also introduce a rule representation for selective explanations. We present efficient methods for computing selective explanations based on a query rewriting method for existential rules. Experimental results on our prototype system shows that our system can scale over very large datasets, and the generated explanations can be significantly reduced in practice. Moreover, we also show some sample explanations on a NLP question answering benchmark, which shows the potential of applying our explanations in question answering.

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