Extending the Combined Approach Beyond Lightweight Description Logics*

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Abstract. Combined approaches have become a successful technique for CQ answering over ontologies. Existing algorithms, however, are restricted to the logics underpinning the OWL 2 profiles. Our goal is to make combined approaches applicable to a wider range of ontologies. We focus on RSA: a class of Horn ontologies that extends the profiles while ensuring tractability of standard reasoning. We show that CQ answering over RSA ontologies without role composition is feasible in NP. Our reasoning procedure generalises the combined approach for $\mathcal{ELHO}$ and DL-Lite$_\mathcal{R}$ using an encoding of CQ answering into fact entailment w.r.t. a logic program with function symbols and stratified negation. Our results are significant in practice since many out-of-profile Horn ontologies are RSA.

1 Introduction

Answering conjunctive queries (CQs) over ontology-enriched datasets is a core reasoning task in many applications. CQ answering is computationally expensive: for expressive description logics it is at least doubly exponential in combined complexity [10], and it remains single exponential even when restricted to Horn ontologies [15].

Recently, there has been a growing interest in ontology languages with favourable computational properties, such as $\mathcal{EL}$ [1], DL-Lite [2] or the rule language datalog, which underpin the EL, QL and RL profiles of OWL 2 [13], respectively. Standard reasoning tasks (e.g., satisfiability checking) are tractable for all three profiles. CQ answering is NP-complete (in combined complexity) for the QL and RL profiles, and PSPACE-complete for OWL 2 EL [18]; PSPACE-hardness of CQ answering in EL is due to role composition axioms and the complexity further drops to NP if these are restricted to express role transitivity and reflexivity [16]. Furthermore, in all these cases CQ answering is tractable in data complexity. Such complexity bounds are rather benign, and this has spurred the development of a wide range of practical algorithms.

A technique that is receiving increasing attention is the *combined approach* [12, 7, 8, 11, 17]. Data is augmented in a query-independent way to build (in polynomial time) a canonical interpretation that might not be a model, but that can be exploited for CQ answering in two alternative ways: either the query is rewritten and then evaluated against

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the interpretation [7] or the query is first evaluated over the interpretation and unsound answers are discarded by means of a *filtration* process [17, 11]. With the exception of [5] and [19] who focus on decidable classes of existential rules, algorithms based on the combined approach are restricted to (fragments of) the OWL 2 profiles.

Our goal is to push the boundaries of the logics underpinning the OWL 2 profiles while retaining their nice complexity for CQ answering. Furthermore, we aim to devise algorithms that seamlessly extend the combined approach and which can be applied to a wide range of ontologies.

Recently, a class of Horn ontologies, called *role safety acyclic* (RSA), has been proposed [3, 4]. RSA extends the profiles while ensuring tractability of standard reasoning tasks: it allows the use of all language constructs in the profiles, while establishing polynomially checkable conditions that preclude their harmful interaction. Roles in an RSA ontology are partitioned into *safe* and *unsafe* depending on the way they are used, where the latter ones are involved in potentially harmful interactions which could increase complexity; an *acyclicity* condition is imposed on unsafe roles to ensure tractability. A recent evaluation revealed that over 60% of out-of-profile Horn ontologies are RSA [4].

In this paper, we investigate CQ answering over RSA ontologies and show its feasibility in NP. This result has significant implications in practice as it shows that CQ answering over a wide range of out-of-profile ontologies is no harder (in combined complexity) than over a database. Our procedure generalises the combined approach for $\mathcal{ELHO}$ [17] and DL-Lite$_{\mathcal{R}}$ [11] in a seamless way by means of a declarative encoding of CQ answering into fact entailment w.r.t. a logic program (LP) with function symbols and stratified negation. The least Herbrand model of this program can be computed in time polynomial in the ontology size and exponential in query size. We have implemented our encoding using the LP engine DLV [9] and tested its feasibility with encouraging results. Proofs can be found online at `http://tinyurl.com/pqmxa5u`.

2 Preliminaries

Logic Programs We use the standard notions of constants, terms, and atoms in first-order logic (FO). A *literal* is an atom a or its negation $not\ a$. A rule r is an expression of the form $\varphi(\vec{x}, \vec{z}) \to \psi(\vec{x})$ with $\varphi(\vec{x}, \vec{z})$ a conjunction of literals with variables $\vec{x} \cup \vec{z}$, and $\psi(\vec{x})$ a non-empty conjunction of atoms over $\vec{x}$.[3] We denote with $vars(r)$ the set $\vec{x} \cup \vec{z}$. With $head(r)$ we denote the set of atoms in ψ, $body^+(r)$ is the set of atoms in φ, and $body^-(r)$ is the set of atoms which occur negated in r. Rule r is safe if each variable in $vars(r)$ occurs in $body^+(r)$; in this paper we consider only safe rules. Rule r is *definite* if $body^-(r)$ is empty and it is *datalog* if it is definite and function-free. A *fact* is a rule with empty body and head consisting of a single function-free atom.

A program $\mathcal{P}$ is a finite set of rules. Let $preds(X)$ denote the predicates in X, with X a (set of) atoms or a program. A *stratification* of $\mathcal{P}$ is a function $str : preds(\mathcal{P}) \to \{1, \ldots, k\}$, where $k \leq |preds(\mathcal{P})|$, s.t. for every $r \in \mathcal{P}$ and $P \in preds(head(r))$ it holds that: *(i)* for every $Q \in preds(body^+(r))$: $str(Q) \leq str(P)$, and *(ii)* for every $Q \in preds(body^-(r))$: $str(Q) < str(P)$. The *stratification partition* of $\mathcal{P}$ induced

[3] We assume rule heads non-empty, and allow multiple atoms.

by str is the sequence $(\mathcal{P}_1, \ldots, \mathcal{P}_k)$, with $\mathcal{P}_i$ consisting of all rules $r \in \mathcal{P}$ such that $max_{a \in head(r)}(str(pred(a))) = i$. The programs $\mathcal{P}_i$ are the *strata* of P. A program is *stratified* if it admits a stratification. All definite programs are stratified.

Stratified programs have a least Herbrand model (LHM), which is constructed using the immediate consequence operator $T_{\mathcal{P}}$. Let $\mathbf{U}$ and $\mathbf{B}$ be the Herbrand universe and base of $\mathcal{P}$, resp., and let $S \subseteq \mathbf{B}$. Then, $T_{\mathcal{P}}(S)$ consists of all facts in $head(r)\sigma$ with $r \in \mathcal{P}$ and σ a substitution from $vars(r)$ to $\mathbf{U}$ satisfying $body^+(r)\sigma \subseteq S$ and $body^-(r)\sigma \cap S = \emptyset$. The powers of $T_{\mathcal{P}}$ are as follows: $T^0_{\mathcal{P}}(S) = S$, $T^{i+1}_{\mathcal{P}}(S) = T_{\mathcal{P}}(T^n_{\mathcal{P}}(S))$, and $T^{\omega}_{\mathcal{P}}(S) = \bigcup_{i=0}^{\infty} T^n_{\mathcal{P}}(S)$. Let str be a stratification of $\mathcal{P}$, and let $(\mathcal{P}_1, \ldots, \mathcal{P}_k)$ be its stratification partition. Also, let $U_1 = T^{\omega}_{\mathcal{P}_1}(\emptyset)$ and for each $1 \leq i \leq k$ let $U_{i+1} = T^{\omega}_{\mathcal{P}_{i+1}}(U_i)$. Then, the LHM of $\mathcal{P}$ is U_k and is denoted $M[\mathcal{P}]$. A program $\mathcal{P}$ entails a positive existential sentence α ($\mathcal{P} \models \alpha$) if $M[\mathcal{P}]$ seen as a FO structure satisfies α.

We use LPs to encode FO theories. For this, we introduce rules axiomatising the built-in semantics of the equality ($\approx$) and truth ($\top$) predicates. For a finite signature Σ, we denote with $\mathcal{F}^{\top}_{\Sigma}$ the smallest set with a rule $p(x_1, x_2, \ldots, x_n) \to \top(x_1) \wedge \top(x_2) \wedge \ldots \wedge \top(x_n)$ for each n-ary predicate p in Σ, and with $\mathcal{F}^{\approx}_{\Sigma}$ the usual axiomatisation of $\approx$ as a congruence over Σ. For an LP $\mathcal{P}$, we denote with $\mathcal{P}^{\approx,\top}$ the extension of $\mathcal{P}$ to $\mathcal{P} \cup \mathcal{F}^{\top}_{\Sigma} \cup \mathcal{F}^{\approx}_{\Sigma}$ with Σ the signature of $\mathcal{P}$.

Ontologies and Queries We define Horn-$\mathcal{ALCHOIQ}$ and specify its semantics via translation to definite programs. W.l.o.g. we consider a normal form close to that in [14]. Let N_{C}, N_{R} and N_{I} be countable pairwise disjoint sets of concept names, role names and individuals. We assume $\{\top, \bot\} \subseteq N_{\mathsf{C}}$. A *role* is an element of $N_{\mathsf{R}} \cup \{R^- | R \in N_{\mathsf{R}}\}$, where the roles in the latter set are called *inverse roles*. The function $\mathsf{Inv}(\cdot)$ is defined as follows, where $R \in N_{\mathsf{R}}$: $\mathsf{Inv}(R) = R^-$ and $\mathsf{Inv}(R^-) = R$. An *RBox* $\mathcal{R}$ is a finite set of axioms (R2) in Table 1, where R and S are roles; $\sqsubseteq^*_{\mathcal{R}}$ is the minimal reflexive-transitive relation over roles s.t. $\mathsf{Inv}(R) \sqsubseteq^*_{\mathcal{R}} \mathsf{Inv}(S)$ and $R \sqsubseteq^*_{\mathcal{R}} S$ hold if $R \sqsubseteq S \in \mathcal{R}$. A *TBox* $\mathcal{T}$ is a finite set of axioms (T1)-(T5) where $A, B \in N_{\mathsf{C}}$ and R is a role.[4] An *ABox* $\mathcal{A}$ is a finite set of axioms of the form (A1) and (A2), with $A \in N_{\mathsf{C}}$ and $R \in N_{\mathsf{R}}$. An *ontology* is a finite set of axioms $\mathcal{O} = \mathcal{R} \cup \mathcal{T} \cup \mathcal{A}$.

OWL 2 specifies the EL, QL, and RL profiles, which are all fragments of Horn-$\mathcal{ALCHOIQ}$ with the exception of property chain axioms and transitivity, which we do not consider here. An ontology is: *(i) EL* if it does not contain inverse roles or axioms (T4); *(ii) RL* if it does not contain axioms (T5); and *(iii) QL* if it does not contain axioms (T2) or (T4), each axiom (T1) satisfies $n = 1$, and each axiom (T3) satisfies $A = \top$.

A *conjunctive query (CQ)* Q is a formula $\exists \vec{y}.\psi(\vec{x}, \vec{y})$ with $\psi(\vec{x}, \vec{y})$ a non-empty conjunction of function-free atoms over $\vec{x} \cup \vec{y}$, where $\vec{x}$ are the *answer variables*. We denote with $terms(Q)$ the set of terms in Q. Queries with no answer variables are *Boolean* (BCQs) and for convenience are written as a set of atoms.

We define the semantics by a mapping π into definite rules as in Table 1 and let $\pi(\mathcal{O}) = \{\pi(\alpha) \mid \alpha \in \mathcal{O}\}$ [5]. An ontology $\mathcal{O}$ is satisfiable if $\pi(\mathcal{O})^{\approx,\top} \not\models \exists y.\bot(y)$. A tuple of constants $\vec{c}$ is an *answer* to Q if $\mathcal{O}$ is unsatisfiable, or $\pi(\mathcal{O})^{\approx,\top} \models \exists \vec{y}.\psi(\vec{c}, \vec{y})$. The set of answers is written $cert(Q, \mathcal{O})$. This semantics is equivalent to the usual one.

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[4] Axioms $A \sqsubseteq \geq n\, R.B$ can be simulated by (T1) and (T5).

[5] By abuse of notation we say that $R^- \in \mathcal{O}$ whenever R^- occurs in $\mathcal{O}$.

	Axioms α	Definite LP rules $\pi(\alpha)$
(R1)	R^-	$R(x,y) \to R^-(y,x); R^-(y,x) \to R(x,y)$
(R2)	$R \sqsubseteq S$	$R(x,y) \to S(x,y)$
(T1)	$\bigsqcap_{i=1}^n A_i \sqsubseteq B$	$\bigwedge_{i=1}^n A_i(x) \to B(x)$
(T2)	$A \sqsubseteq \{a\}$	$A(x) \to x \approx a$
(T3)	$\exists R.A \sqsubseteq B$	$R(x,y) \wedge A(y) \to B(x)$
(T4)	$A \sqsubseteq \leq 1R.B$	$A(x) \wedge R(x,y) \wedge B(y) \wedge R(x,z) \wedge B(z) \to y \approx z$
(T5)	$A \sqsubseteq \exists R.B$	$A(x) \to R(x, f_{R,B}^A(x)) \wedge B(f_{R,B}^A(x))$
(A1)	$A(a)$	$\to A(a)$
(A2)	$R(a,b)$	$\to R(a,b)$

Table 1: Translation from Horn ontologies into rules.

3 Reasoning over RSA Ontologies

CQ answering is ExpTime-complete for Horn-$\mathcal{ALCHOIQ}$ ontologies [14], and the ExpTime lower bound holds already for satisfiability checking. Intractability is due to *and-branching*: owing to the interaction between axioms in Table 1 of type (T5) with either axioms (T3) and (R1), or axioms (T4) an ontology may only be satisfied by large (possibly infinite) models which cannot be succinctly represented.

RSA is a class of ontologies where all axioms in Table 1 are allowed, but their interaction is restricted s.t. model size can be polynomially bounded [4]. We recapitulate RSA ontologies and their properties; let $\mathcal{O}$ be an arbitrary Horn-$\mathcal{ALCHOIQ}$ ontology.

Roles in $\mathcal{O}$ are divided into *safe* and *unsafe*. The intuition is that unsafe roles may participate in harmful interactions.

Definition 1. *A role R is* unsafe *if it occurs in an axiom of the form $A \sqsubseteq \exists R.B$, and there is a role S s. t. either: 1. $R \sqsubseteq_{\mathcal{R}}^* \mathsf{Inv}(S)$ and S occurs in an axiom of the form $\exists S.A \sqsubseteq B$ with $A \neq \top$, or 2. $R \sqsubseteq_{\mathcal{R}}^* S$ or $R \sqsubseteq_{\mathcal{R}}^* \mathsf{Inv}(S)$ and S occurs in an axiom of the form $A \sqsubseteq \leq 1S.B$. A role R in $\mathcal{O}$ is* safe*, if it is not unsafe.*

It follows from Definition 1 that RL, QL, and EL ontologies contain only safe roles.

Example 1. Let $\mathcal{O}_{\mathsf{Ex}}$ be the (out-of-profile) ontology with the following axioms:

$$A(a) \quad (1) \qquad A \sqsubseteq \exists S^-.C \quad (3) \qquad D \sqsubseteq \exists R.B \quad (5) \qquad R \sqsubseteq T^- \quad (7)$$
$$A \sqsubseteq D \quad (2) \qquad \exists S.A \sqsubseteq D \quad (4) \qquad B \sqsubseteq \exists S.D \quad (6) \qquad S \sqsubseteq T \quad (8)$$

Roles R, S, T, and T^- are safe; however, S^- is unsafe as it occurs in an axiom (T5) while S occurs in an axiom (T3). We will $\mathcal{O}_{\mathsf{Ex}}$ use as a running example.

The distinction between safe and unsafe roles makes it possible to strengthen the translation π in Table 1 while preserving satisfiability and entailment of unary facts. The translation of axioms (T5) with R safe can be realised by replacing the functional term $f_{R,B}^A(x)$ with a Skolem constant $v_{R,B}^A$ unique to A, R and B. The modified transformation generally leads to a smaller LHM: if all roles are safe then $\mathcal{O}$ is mapped into a datalog program whose LHM is polynomial in the size of $\mathcal{O}$.

Definition 2. *Let $v^A_{R,B}$ be a fresh constant for each concept A, B, and each safe role R in $\mathcal{O}$. Then π_{safe} maps each $\alpha \in \mathcal{O}$ to (i) $A(x) \to R(x, v^A_{R,B}) \wedge B(v^A_{R,B})$ if α is of type (T5) with R safe; (ii) $\pi(\alpha)$, otherwise. Let $\mathcal{P} = \{\pi_{\mathsf{safe}}(\alpha) \mid \alpha \in \mathcal{O}\}$ and $\mathcal{P}_{\mathcal{O}} = \mathcal{P}^{\approx,\top}$.*

Example 2. Mapping π_{safe} differs from π on axiom (5) and (6). For instance, (5) yields $D(x) \to R(x, v^D_{R,B}) \wedge B(v^D_{R,B})$.

Theorem 1. *[4, Theorem 2] Ontology $\mathcal{O}$ is satisfiable iff $\mathcal{P}_{\mathcal{O}} \not\models \exists y.\bot(y)$. If $\mathcal{O}$ is satisfiable, then $\mathcal{O} \models A(c)$ iff $A(c) \in M[\mathcal{P}_{\mathcal{O}}]$ for all $A \in N_{\mathsf{C}}$ and $c \in N_{\mathsf{I}}$ from $\mathcal{O}$.*

If $\mathcal{O}$ has unsafe roles the model $M[\mathcal{P}_{\mathcal{O}}]$ might be infinite. We next define a datalog program $\mathcal{P}_{\mathsf{RSA}}$ by introducing Skolem constants for all axioms (T5) in $\mathcal{O}$. $\mathcal{P}_{\mathsf{RSA}}$ introduces also a predicate PE which 'tracks' all binary facts generated by the application of Skolemised rules over unsafe roles. A unary predicate U is initialised with the constants associated to unsafe roles and a rule $\mathsf{U}(x) \wedge \mathsf{PE}(x, y) \wedge \mathsf{U}(y) \to \mathsf{E}(x, y)$ stores the PE-facts originating from unsafe roles using a predicate E. Then, $M[\mathcal{P}_{\mathcal{O}}]$ is of polynomial size when the graph induced by the extension of E is an oriented forest (i.e., a DAG whose underlying undirected graph is a forest). When this condition is fulfilled together with some additional conditions which preclude harmful interactions between equality-generating axioms and inverse roles, we say that $\mathcal{O}$ is RSA.

Definition 3. *Let PE and E be fresh binary predicates, U be a fresh unary predicate, and $u^A_{R,B}$ be a fresh constant for each concept A, B and each role R in $\mathcal{O}$. Function π_{RSA} maps each (i) $\alpha \in \mathcal{O}$ to $A(x) \to R(x, u^A_{R,B}) \wedge B(u^A_{R,B}) \wedge \mathsf{PE}(x, u^A_{R,B})$, if α is of type (T5), and to (ii) $\pi(\alpha)$, otherwise. Let $\mathcal{P}_{\mathsf{RSA}}$ be the smallest program that contains $\pi_{\mathsf{RSA}}(\alpha)$ for each $\alpha \in \mathcal{O}$, and a rule $\mathsf{U}(x) \wedge \mathsf{PE}(x, y) \wedge \mathsf{U}(y) \to \mathsf{E}(x, y)$ and a fact $\mathsf{U}(u^A_{R,B})$ for each $u^A_{R,B}$ with R unsafe.*

Let M_{RSA} be the LHM of $\mathcal{P}_{\mathsf{RSA}}{}^{\approx,\top}$. Then, $G_{\mathcal{O}}$ is the digraph with an edge (c, d) for each $\mathsf{E}(c, d)$ in M_{RSA}. Ontology $\mathcal{O}$ is equality-safe if: 1. for each pair of atoms $w \approx t$ (with w and t distinct) and $R(t, u^A_{R,B})$ in M_{RSA} and each role S s.t. $R \sqsubseteq \mathsf{Inv}(S)$, it holds that S does not occur in an axiom (T4); and 2. for each pair of atoms $R(a, u^A_{R,B}), S(u^A_{R,B}, a)$ in M_{RSA}, with $a \in N_{\mathsf{I}}$, there does not exist a role T such that both $R \sqsubseteq^*_{\mathcal{R}} T$ and $S \sqsubseteq^*_{\mathcal{R}} \mathsf{Inv}(T)$ hold.

We say that $\mathcal{O}$ is RSA if it is equality-safe and $G_{\mathcal{O}}$ is an oriented forest.

The fact that $G_{\mathcal{O}}$ is a DAG ensures that the LHM $M[\mathcal{P}_{\mathcal{O}}]$ is finite, whereas the lack of 'diamond-shaped' subgraphs in $G_{\mathcal{O}}$ guarantees polynomiality of $M[\mathcal{P}_{\mathcal{O}}]$. The safety condition on $\approx$ will ensure that RSA ontologies enjoy a special form of forest-model property that we exploit for CQ answering. Every ontology in QL (which is equality-free), RL (where $\mathcal{P}_{\mathsf{RSA}}$ has no Skolem constants) and EL (no inverse roles) is RSA.

Theorem 2. *[4, Theorem 3] If $\mathcal{O}$ is RSA, then $|M[\mathcal{P}_{\mathcal{O}}]|$ is polynomial in $|\mathcal{O}|$.*

Tractability of standard reasoning for RSA ontologies follows from Theorems 1 and 2. While the ontology $\mathcal{O}_{\mathsf{Ex}}$ from Example 1 cannot be captured by any of the profiles of OWL 2, it can be checked that $\mathcal{O}_{\mathsf{Ex}}$ is RSA.

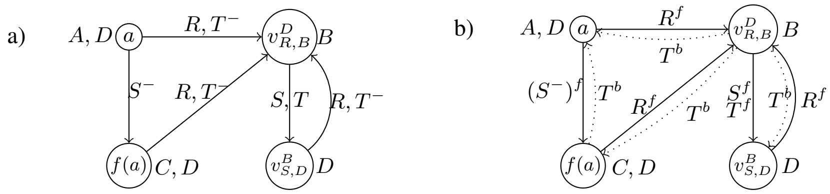

Fig. 1: Original (a) and annotated (b) model for $\mathcal{O}_{\mathsf{Ex}}$

4 Answering Queries over RSA Ontologies

We next present our combined approach with filtration to CQ answering over RSA ontologies, which generalises existing techniques for DL-Lite$_\mathcal{R}$ and $\mathcal{ELHO}$.

In Section 4.1 we take the LHM for RSA ontologies given in Section 3 as a starting point and extend it to a more convenient canonical model over an extended signature. In order to deal with the presence of inverse roles in RSA ontologies, the extended model captures the "directionality" of binary atoms; this will allow us to subsequently extend the filtration approach from [17] in a seamless way. The canonical model is captured declaratively as the LHM of a logic program over the extended signature.

As usual in combined approaches, this model is not universal and the evaluation of CQs may lead to spurious, i.e. unsound answers. In Section 4.2, we specify our filtration approach for RSA ontologies as the LHM of a stratified program. In the following, we fix an arbitrary RSA ontology $\mathcal{O} = \mathcal{R} \cup \mathcal{T} \cup \mathcal{A}$ and an input CQ Q, which we use to parameterise all our technical results.

4.1 Constructing the Canonical Model

The LHM $M[\mathcal{P}_\mathcal{O}]$ in Section 3 is a model of $\mathcal{O}$ that preserves entailment of unary facts. It generalises the canonical model in [17], which is specified as the LHM of a datalog program obtained by Skolemising all axioms (T5) into constants and hence coincides with $M[\mathcal{P}_\mathcal{O}]$ when $\mathcal{O}$ is EL. However, RSA ontologies allow for unsafe roles and hence $M[\mathcal{P}_\mathcal{O}]$ may contain also functional terms.

A main source for spurious matches when evaluating Q over the canonical model of an EL ontology is the presence of 'forks'—confluent chains of binary atoms—in the query which map to 'forks' in the model over Skolem constants. This is also problematical in our setting since RSA ontologies have the forest-model property.

Example 3. Fig. 1.a) depicts the LHM $M[\mathcal{P}_{\mathcal{O}_{\mathsf{Ex}}}]$ of $\mathcal{O}_{\mathsf{Ex}}$ (the function symbol $f_{S,C}$ is abbreviated with f). We see models as digraphs where the direction of edges reflects the satisfaction of axioms (T5). Consider $Q_1 = \{A(y_1), R(y_1, y_2), R(y_3, y_2)\}$. Substitution $(y_1 \mapsto a, y_2 \mapsto v^D_{R,B}, y_3 \mapsto v^B_{S,D})$ is a spurious match of Q_1 as it relies on edges $(a, v^D_{R,B})$ and $(v^B_{S,D}, v^D_{R,B}))$ in $M[\mathcal{P}_{\mathcal{O}_{\mathsf{Ex}}}]$, which form a fork over $v^D_{R,B}$.

In EL, only queries which contain forks can be mapped to forks in the model. This is no longer the case for RSA ontologies, where forks in the model can lead to spurious answers even for linearly-shaped queries due to the presence of inverse roles.

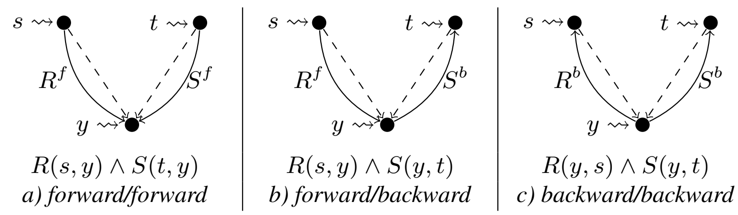

Fig. 2: Forks in the presence of inverse roles

Example 4. Let $Q_2 = \{A(y_1), R(y_1, y_2), T(y_2, y_3)\}$. Then $(y_1 \mapsto a, y_2 \mapsto v^D_{R,B}, y_3 \mapsto f(a))$ is a spurious match for Q_2 as it relies on the fork $(a, v^D_{R,B})$, $(f(a), v^D_{R,B})$. Axiom $R \sqsubseteq T^-$ causes a linear match over R and T to become a fork over R and T^-.

To identify such situations, we compute a canonical model over an extended signature that contains fresh roles R^f and R^b for each role R. Annotations f (forward) and b (backwards) are intended to reflect the directionality of binary atoms in the model, where binary atoms created to satisfy an axiom (T5) are annotated with f. To realise this intuition declaratively, we modify the rules in $\mathcal{P}_\mathcal{O}$ for axioms (T5) as follows. If R is safe, then we introduce the rule $A(x) \to R^f(x, v^A_{R,B}) \wedge B(v^A_{R,B})$; if it is unsafe, we introduce rule $A(x) \to R^f(x, f^A_{R,B}(x)) \wedge B(f^A_{R,B})$ instead.

Superroles inherit the direction of the subrole, while roles and their inverses have opposite directions. To reflect this we include the following rules where $* \in \{f, b\}$: *(i)* $R^*(x, y) \to S^*(x, y)$ for each axiom $R \sqsubseteq S$ in $\mathcal{O}$; *(ii)* $R^f(x, y) \to \mathsf{Inv}(R)^b(y, x)$ and $R^b(x, y) \to \mathsf{Inv}(R)^f(y, x)$ for each role R; and *(iii)* $R^*(x, y) \to R(x, y)$ for each role R. Rules *(ii)* are included only if $\mathcal{O}$ has inverse roles, and rules *(iii)* 'copy' annotated atoms to atoms over the original predicate. Fig. 1.b) shows the annotated model for $P_{\mathcal{O}_{\mathsf{Ex}}}$: solid (resp. dotted) lines represent 'forward' (resp. 'backward') atoms.

Fig. 2 depicts the ways in which query matches may spuriously rely on a fork in an annotated model. Nodes represent the images in the model of the query terms; solid lines indicate the annotated atoms responsible for the match; and dashed lines depict the underpinning fork. The images of s and t must not be equal; additionally, y cannot be mapped to (a term identified to) a constant in $\mathcal{O}$. For instance, the match in Ex. 4 is spurious as it corresponds to pattern (b) in Fig. 2. Unfortunately, the annotated model can present ambiguity: it is possible for both atoms $R^f(s, t)$ and $R^b(s, t)$ to hold.

Example 5. Consider Q_2 from Ex. 4. $(y_1 \mapsto a, y_2 \mapsto v^D_{R,B}, y_3 \mapsto v^B_{S,D})$ is also a match, where both $T^f(v^D_{R,B}, v^B_{S,D})$ and $T^b(v^D_{R,B}, v^B_{S,D})$ hold in the annotated model.

Such ambiguity is problematic for the subsequent filtration step. To disambiguate, we use a technique similar to the one in [11] for DL-Lite$_\mathcal{R}$, where the idea is to unfold certain cycles of length one and two in the canonical model. We unfold self-loops to cycles of length three while cycles of length two are unfolded to cycles of length four.

Example 6. Fig. 3 a) shows the model expansion for $\mathcal{O}_{\mathsf{Ex}}$. As one can see, the ambiguities are resolved. Fig. 3 b) shows the unfolding of a generic self-loop over a safe role R for which T exists s.t. both $R \sqsubseteq^*_\mathcal{R} T$ and $R \sqsubseteq^*_\mathcal{R} \mathsf{Inv}(T)$ hold.

We now specify a program that yields the required model.

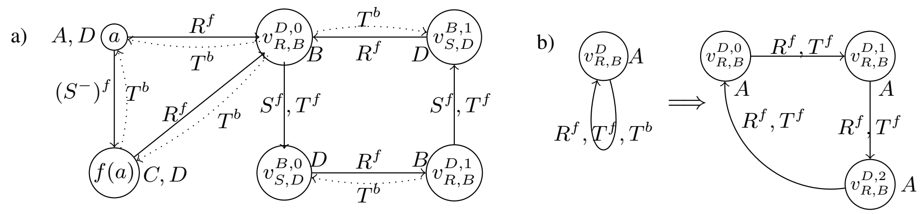

Fig. 3: Model expansion in the presence of loops/cycles

Definition 4. *Let* $\mathsf{confl}(R)$ *be the set of roles* S *s.t.* $R \sqsubseteq^*_{\mathcal{R}} T$ *and* $S \sqsubseteq^*_{\mathcal{R}} \mathsf{Inv}(T)$ *for some* T*. Let* $\prec$ *be a strict total order on triples* (A, R, B)*, with* R *safe and* A *and* B *concept names* B *in* $\mathcal{O}$*. For each* (A, R, B)*, let:*

(i) $v^{A,0}_{R,B}$, $v^{A,1}_{R,B}$, *and* $v^{A,2}_{R,B}$ *be fresh constants;*
(ii) $\mathsf{self}(A, R, B)$ *be the smallest set containing* $v^{A,0}_{R,B}$ *and* $v^{A,1}_{R,B}$ *if* $R \in \mathsf{confl}(R)$*;*
(iii) $\mathsf{cycle}(A, R, B)$ *be the smallest set containing, for each* $S \in \mathsf{confl}(R)$, $v^{D,0}_{S,C}$ *if* $(A, R, B) \prec (D, S, C)$*;* $v^{D,1}_{S,C}$ *if* $(D, S, C) \prec (A, R, B)$*;* $f^{D}_{S,C}(v^{A,0}_{R,B})$ *and every* $f^{F}_{T,E}(v^{A,0}_{R,B})$ *s. t.* $u^{D}_{S,C} \approx u^{F}_{T,E}$ *is in* M_{RSA}*, if* S *is unsafe.*
(iv) $\mathsf{unfold}(A, R, B) = \mathsf{self}(A, R, B) \cup \mathsf{cycle}(A, R, B)$.

Let R^f *and* R^b *be fresh binary predicates for each role* R *in* $\mathcal{O}$*,* NI *be a fresh unary predicate, and* notIn *be a built-in predicate which holds when the first argument is an element of second argument. Let* $\mathcal{P}$ *be the smallest program with a rule* $\rightarrow \mathsf{NI}(a)$ *for each constant* a *and all rules in Fig. 4 and* $E_{\mathcal{O}} = \mathcal{P}^{\approx,\top}$*.*

Symbols/Axioms in $\mathcal{O}$	Logic Programming Rules
ax. α not of type (T5)	$\pi(\alpha)$
$R \sqsubseteq S$, $* \in \{f, b\}$	$R^*(x, y) \rightarrow S^*(x, y)$
R role, $* \in \{f, b\}$	$R^*(x, y) \rightarrow R(x, y)$ $R^f(x, y) \rightarrow \mathsf{Inv}(R)^b(y, x)$ $R^b(x, y) \rightarrow \mathsf{Inv}(R)^f(y, x)$
ax. (T5), R unsafe	$A(x) \rightarrow R^f(x, f^A_{R,B}(x)) \wedge B(f^A_{R,B}(x))$
ax. (T5), R safe	$A(x) \wedge \mathsf{notIn}(x, \mathsf{unfold}(A, R, B)) \rightarrow R^f(x, v^{A,0}_{R,B}) \wedge B(v^{A,0}_{R,B})$
	if $R \in \mathsf{confl}(R)$, for every $i = 0, 1$: $A(v^{A,i}_{R,B}) \rightarrow R^f(v^{A,i}_{R,B}, v^{A,i+1}_{R,B}) \wedge B(v^{A,i+1}_{R,B})$
	for every $x \in \mathsf{cycle}(A, R, B)$: $A(x) \rightarrow R^f(x, v^{A,1}_{R,B}) \wedge B(v^{A,1}_{R,B})$

Fig. 4: Rules in the program $E_{\mathcal{O}}$

The set $\mathsf{confl}(R)$ contains roles that may cause ambiguity in conjunction with R. The ordering $\prec$ determines how cycles are unfolded using auxiliary constants. Each axiom $A \sqsubseteq \exists R.B$ with R safe is Skolemised by default using $v^{A,0}_{R,B}$, except when the axiom applies to a term in $\mathsf{unfold}(A, R, B)$ where we use $v^{A,1}_{R,B}$ or $v^{A,2}_{R,B}$ instead.

(1) $\psi(\vec{x},\vec{y}) \to \mathsf{QM}(\vec{x},\vec{y})$
(2) $\to named(a)$ for each constant a in $\mathcal{O}$
(3a) $\mathsf{QM}(\vec{x},\vec{y}), not\ \mathsf{NI}(y_i) \to \mathsf{id}(\vec{x},\vec{y},i,i)$, for each $1 \leq i \leq \lvert\vec{y}\rvert$ **(3b)** $\mathsf{id}(\vec{x},\vec{y},u,v) \to \mathsf{id}(\vec{x},\vec{y},v,u)$ **(3c)** $\mathsf{id}(\vec{x},\vec{y},u,v) \wedge \mathsf{id}(\vec{x},\vec{y},v,w) \to \mathsf{id}(\vec{x},\vec{y},u,w)$

for all $R(s,y_i)$, $S(t,y_j)$ in Q with $y_i,y_j \in \vec{y}$
 (4a) $R^f(s,y_i) \wedge S^f(t,y_j) \wedge \mathsf{id}(\vec{x},\vec{y},i,j) \wedge not\ s \approx t \to \mathit{fk}(\vec{x},\vec{y})$
 for all $R(s,y_i)$, $S(y_j,t)$ in Q with $y_i,y_j \in \vec{y}$:
 (4b) $R^f(s,y_i) \wedge S^b(y_j,t) \wedge \mathsf{id}(\vec{x},\vec{y},i,j) \wedge not\ s \approx t \to \mathit{fk}(\vec{x},\vec{y})$
 for all $R(y_i,s)$, $S(y_j,t)$ in Q with $y_i,y_j \in \vec{y}$:
 (4c) $R^b(y_i,s) \wedge S^b(y_j,t) \wedge \mathsf{id}(\vec{x},\vec{y},i,j) \wedge not\ s \approx t \to \mathit{fk}(\vec{x},\vec{y})$

for all $R(y_i,y_j)$, $S(y_k,y_l)$ in Q with $y_i,y_j,y_k,y_l \in \vec{y}$:   **(5a)** $R^f(y_i,y_j) \wedge S^f(y_k,y_l) \wedge \mathsf{id}(\vec{x},\vec{y},j,l) \wedge y_i \approx y_k \wedge not\ \mathsf{NI}(y_i) \to \mathsf{id}(\vec{x},\vec{y},i,k)$ **(5b)** $R^f(y_i,y_j) \wedge S^b(y_k,y_l) \wedge \mathsf{id}(\vec{x},\vec{y},j,k) \wedge y_i \approx y_l \wedge not\ \mathsf{NI}(y_i) \to \mathsf{id}(\vec{x},\vec{y},i,l)$ **(5c)** $R^b(y_i,y_j) \wedge S^b(y_l,y_k) \wedge \mathsf{id}(\vec{x},\vec{y},i,l) \wedge y_j \approx y_k \wedge not\ \mathsf{NI}(y_j) \to \mathsf{id}(\vec{x},\vec{y},j,k)$
for each $R(y_i,y_j)$ in Q with $y_i,y_j \in \vec{y}$, and $* \in \{f,b\}$:   **(6)** $R^*(y_i,y_j) \wedge \mathsf{id}(\vec{x},\vec{y},i,v) \wedge \mathsf{id}(\vec{x},\vec{y},j,w) \to AQ^*(\vec{x},\vec{y},v,w)$
(7a) $AQ^*(\vec{x},\vec{y},u,v) \to TQ^*(\vec{x},\vec{y},u,v)$, for each $* \in \{f,b\}$ **(7b)** $AQ^*(\vec{x},\vec{y},u,v) \wedge TQ^*(\vec{x},\vec{y},v,w) \to TQ^*(\vec{x},\vec{y},u,w)$, for each $* \in \{f,b\}$
(8a) $\mathsf{QM}(\vec{x},\vec{y}) \wedge not\ named(x) \to \mathsf{sp}(\vec{x},\vec{y})$, for each $x \in \vec{x}$ **(8b)** $\mathit{fk}(\vec{x},\vec{y}) \to \mathsf{sp}(\vec{x},\vec{y})$ **(8c)** $TQ^*(\vec{x},\vec{y},v,v) \to \mathsf{sp}(\vec{x},\vec{y})$, for each $* \in \{f,b\}$
(9) $\mathsf{QM}(\vec{x},\vec{y}) \wedge not\ \mathsf{sp}(\vec{x},\vec{y}) \to \mathsf{Ans}(\vec{x})$

Table 2: Rules in $\mathcal{P}_Q$. Variables u, v, w from U are distinct.

Theorem 3. *The following holds: (i) $M[E_{\mathcal{O}}]$ is polynomial in $|\mathcal{O}|$ (ii) $\mathcal{O}$ is satisfiable iff $E_{\mathcal{O}} \not\models \exists y.\bot(y)$ (iii) if $\mathcal{O}$ is satisfiable, $\mathcal{O} \models A(c)$ iff $A(c) \in M[E_{\mathcal{O}}]$ and (iv) there are no terms s, t and role R s.t. $E_{\mathcal{O}} \models R^f(s,t) \wedge R^b(s,t)$.*

4.2 Filtering Unsound Answers

We now define a program $\mathcal{P}_Q$ that can be used to eliminate all spurious matches of Q over the annotated model of $\mathcal{O}$. The rules of the program are summarised in Table 2. We will refer to all terms in the model that are not equal to a constant in $\mathcal{O}$ as *anonymous*.

Matches where an answer variable is not mapped to a constant in $\mathcal{O}$ are spurious. We introduce a predicate $named$ and populate it with such constants (rules **(2)**); then, we flag answers as spurious using a rule with negation (rules **(8a)**).

To detect forks we introduce a predicate *fk*, whose definition in datalog encodes the patterns in Fig. 2 (rules **(4)**). If terms s and t in Fig. 2 are existential variables mapping to the same anonymous term, further forks might be recursively induced.

Example 7. Let $Q_3 = \{A(y_1), R(y_1,y_2), T(y_2,y_3), C(y_4), \ R(y_4,y_5), S(y_5,y_3)\}$ be a BCQ over $\mathcal{O}_{\mathsf{Ex}}$, with $(y_1 \mapsto a, y_2 \mapsto v^{D,0}_{R,B}, y_3 \mapsto v^{B,0}_{S,D}, y_4 \mapsto f(a), y_5 \mapsto v^{D,0}_{R,B})$ being its only match over the model in Fig. 3a). The identity of y_2, y_5 induces a fork on the match of $R(y_1,y_2)$ and $R(y_4,y_5)$.

We track identities in the model relative to a match using a fresh predicate id. It is initialised as the minimal congruence relation over the positions of the existential variables in the query which are mapped to anonymous terms (rules **(3)**). Identity is recursively propagated (rules **(5)**). Matches involving forks are marked as spurious by rule **(8b)**.

Spurious matches can also be caused by cycles in the model and query satisfying certain requirements. First, the positions of existential variables of the query must be cyclic when considering also the id relation. Second, the match must involve only anonymous terms. Finally, all binary atoms must have the same directionality.

Example 8. Consider the following BCQs over $\mathcal{O}_{\mathsf{Ex}}$: $Q_4 = \{S(y_1, y_2), R(y_2, y_3), S(y_3, y_4), R(y_4, y_1)\}$, $Q_5 = \{T(y_1, y_2), S(y_2, y_3), R(y_3, y_1)\}$, and $Q_6 = \{S(y_1, y_2), R(y_2, y_3), S(y_3, y_4), R(y_4, y_5)\}$. Then, $(y_1 \mapsto v^{D,0}_{R,B}, y_2 \mapsto v^{B,0}_{S,D}, y_3 \mapsto v^{D,1}_{R,B}, y_4 \mapsto v^{B,1}_{S,D})$ is a match of Q_4 inducing a cycle: all binary atoms are mapped 'forward' and the cycle involves only anonymous terms. In contrast, match $(y_1 \mapsto v^{D,0}_{R,B}, y_2 \mapsto f(a), y_3 \mapsto a)$ over Q_5 does not satisfy the requirements as it involves constant a. Note that Q_4 and Q_5 are cyclic. Q_6 is not cyclic; thus, although the match $(y_1 \mapsto v^{D,0}_{R,B}, y_2 \mapsto v^{B,0}_{S,D}, y_3 \mapsto v^{D,1}_{R,B}, y_4 \mapsto v^{B,1}_{S,D}, y_5 \mapsto v^{D,0}_{R,B})$ involves a cycle in the model, it is not spurious.

Such cycles are recognised by rules **(6)** and **(7)**. Rule **(6)** defines potential individual arcs in the cycle with their directionality using fresh predicates AQ^* with $* \in \{f, b\}$. Rules **(7)** detect the cycles recursively using predicates TQ^*. Matches involving cycles are marked as spurious by rules **(8c)**. All correct answers are collected by rule **(9)** using predicate Ans. We next define program $\mathcal{P}_Q$ and its extension $\mathcal{P}_{\mathcal{O},Q}$ with $E_{\mathcal{O}}$ in Def. 4, which can be exploited to answer Q w.r.t. $\mathcal{O}$.

Definition 5. *Let $Q = \exists \vec{y}.\psi(\vec{x}, \vec{y})$ be a CQ, let* QM, sp, *and fk be fresh predicates of arity $|\vec{x}| + |\vec{y}|$, let* id, *AQ^*, and TQ^*, with $* \in \{f, b\}$, be fresh predicates of arity $|\vec{x}| + |\vec{y}| + 2$, let* Ans *be a fresh predicate of arity $|\vec{x}|$, let $named$ be a fresh unary predicate, and let U be a set of fresh variables s.t. $|U| \geq |\vec{y}|$. Then, $\mathcal{P}_Q$ is the smallest program with all rules in Table 2, and $\mathcal{P}_{\mathcal{O},Q}$ is defined as $E_{\mathcal{O}} \cup \mathcal{P}_Q$.*

Note that, to distinguish between constants in $\mathcal{O}$ (recorded by $named$ in $\mathcal{P}_Q$) and their closure under equality (recorded by NI in $E_{\mathcal{O}}$), we do not axiomatise equality w.r.t. $\mathcal{P}_Q$.

Theorem 4. *(i) $\mathcal{P}_{\mathcal{O},Q}$ is stratified; (ii) $M[\mathcal{P}_{\mathcal{O},Q}]$ is polynomial in $|\mathcal{O}|$ and exponential in $|Q|$; and (iii) if $\mathcal{O}$ is satisfiable, $\vec{x} \in cert(Q, \mathcal{O})$ iff $\mathcal{P}_{\mathcal{O},Q} \models \mathsf{Ans}(\vec{x})$.*

Theorem 4 suggests a worst-case exponential algorithm that, given $\mathcal{O}$ and Q, materialises $\mathcal{P}_{\mathcal{O},Q}$ and returns the extension of predicate Ans. This procedure can be modified to obtain a 'guess and check' algorithm applicable to BCQs. This algorithm first materialises $E_{\mathcal{O}}$ in polynomial time; then, it guesses a match σ to Q over the materialisation; finally, it materialises $(\mathcal{P}_{\mathcal{O},Q})\sigma$, where variables $\vec{x}$ and $\vec{y}$ are grounded by σ. The latter step can also be shown to be tractable.

Theorem 5. *Checking whether $\mathcal{O} \models Q$ is* NP*-complete in combined complexity.*

5 Proof of Concept

We implemented our approach using the DLVsystem,[6] which supports function symbols and stratified negation. For testing, we used the LUBM ontology [6] (which contains only safe roles) and the Horn fragments of the Reactome and Uniprot (which are

[6] http://www.dlvsystem.com/dlv/

Ontology	Facts (M1)	Model M2/M3	q_1(M4/M5/M6)	q_2(M4/M5/M6)	q_3(M4/M5/M6)	q_4(M4/M5/M6)
Reactome	$54{\cdot}10^3$	8s / $242{\cdot}10^3$	6s / 10 / 0%	5s / 11 / 0%	6s / 50 / 48%	
	$107{\cdot}10^3$	16s / $485{\cdot}10^3$	14s / 11 / 0%	14s / 17 / 0%	12s / 122 / 38%	
	$159{\cdot}10^3$	21s / $728{\cdot}10^3$	42s / 17 / 0%	44s / 23 / 0%	36s/ 216 / 35%	
	$212{\cdot}10^3$	19s / $970{\cdot}10^3$	19s / 21 / 0%	15s/ 24 / 0%	14s/ 299 / 34%	
LUBM	$37{\cdot}10^3$	4s / $213{\cdot}10^3$	11s / 2350 / 86%	4s / 650/ 96%	4s / 1580/ 0%	5s / 1743/ 0%
	$75{\cdot}10^3$	6s / $395{\cdot}10^3$	45s / 9340/ 85%	8s / 1640/ 97%	9s / 7925/ 0%	8s / 5969/ 0%
	$113{\cdot}10^3$	8s / $550{\cdot}10^3$	108s / 24901/ 83%	13s / 2352/ 98%	13s / 18661/ 0%	13s / 10870/ 0%
	$150{\cdot}10^3$	11s / $682{\cdot}10^3$	188s / 52196/ 83%	17s / 2550/ 98%	18s / 32370/ 0%	24s / 15076/ 0%
	$188{\cdot}10^3$	12s / $795{\cdot}10^3$	305s / 91366/ 82%	31s / 2550/ 98%	40s / 49555/ 0%	38s / 18517/ 0%
	$226{\cdot}10^3$	14s / $894{\cdot}10^3$	390s / 148340/ 80%	39s / 2550/ 98%	46s / 72438/ 0%	40s / 20404/ 0%
Uniprot	$10{\cdot}10^3$	1s / $51{\cdot}10^3$	1s / 2 / 0%	1s / 0 / 0%	1s / 18 / 28%	
	$49{\cdot}10^3$	4s / $246{\cdot}10^3$	3s / 7 / 0%	3s / 0 / 0%	3s / 89 / 26%	
	$98{\cdot}10^3$	9s / $487{\cdot}10^3$	7s / 9 / 0%	6s / 1 / 0%	6s / 193 / 23%	
	$146{\cdot}10^3$	11s / $726{\cdot}10^3$	13s / 14 / 0%	12s / 1 / 0%	10s / 273 / 22%	

Table 3: Evaluation Results

RSA, but contain also unsafe roles).[7] LUBM comes with a data generator; Reactome and Uniprot come with large datasets, which we sampled. Test queries are given in the appendix. We measured (M1) number of facts of the given data; (M2) materialisation times for the canonical model; (M3) model size; (M4) materialisation times for $\mathcal{P}_Q$; (M5) number of candidate query answers; and (M6) percentage of spurious answers. Experiments were performed on a MacBook Pro laptop with 8GB RAM and an Intel Core 2.4 GHz processor.

Table 3 summarises our results. Computation times for the models scale linearly in data size. Model size is at most 6 times larger than the original data, which is a reasonable growth factor in practice. As usual in combined approaches (e.g. see [17]), query processing times depend on the number of candidate answers; thus, the applicability of the approach largely depends on the ratio between spurious and correct answers. Queries q_1-q_2 in Reactome and Uniprot are realistic queries given as examples in the EBI website. Neither of these queries lead to spurious answers, and processing times scale linearly with data size. No query in the LUBM benchmark leads to spurious answers (e.g., LUBM queries q_3 and q_4 in Table 3). We manually crafted one additional query for Reactome and Uniprot (q_3 in both cases) and two for LUBM (queries q_1 and q_2), which lead to a high percentage of spurious answers. Although these queries are challenging, we can observe that the proportion of spurious answers remains constant with increasing data size. Finally, note that query q_1 in LUBM retrieves the highest number of candidate answers and is thus the most challenging query. Our prototype and all test data, ontologies and queries are available at http://tinyurl.com/qcolx3w.

6 Conclusions and Future Work

We presented an extension to the combined approaches to CQ answering that can be applied to a wide range of out-of-profile Horn ontologies. Our theoretical results unify and extend existing techniques for $\mathcal{ELHO}$ and DL-Lite$_\mathcal{R}$ in a seamless and elegant way. Our preliminary experiments indicate the feasibility of our approach in practice.

We anticipate several directions for future work. First, we have not considered logics with transitive roles. Recently, it was shown that CQ answering over EL ontologies with

[7] http://www.ebi.ac.uk/rdf/platform

transitive roles is feasible in NP [16]. We believe that our techniques can be extended in a similar way. Finally, we would like to optimise our encoding into LP and conduct a more extensive evaluation.

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Appendix

Queries Used for Proof of Concept

Reactome queries:
q_1 : {$\mathsf{Pathway}(y_1), \mathsf{pathwayComponent}(y_1, y_2), \mathsf{BiochemicalReaction}(y_2),$ $\mathsf{participant}(y_2, y_3), \mathsf{Protein}(y_3)$}
q_2 : {$\mathsf{Pathway}(y_1), \mathsf{pathwayComponent}(y_1, y_2), \mathsf{BiochemicalReaction}(y_2),$ $\mathsf{participant}(y_2, y_3), \mathsf{Complex}(y_3)$}
q_3 : {$\mathsf{participantStoichiometry}(y_1, y_2), \mathsf{physicalEntity}(y_2, y_3),$ $\mathsf{participantStoichiometry}(y_3, y_4), \mathsf{physicalEntity}(y_4, y_3)$}
LUBM queries:
q_1 : {$\mathsf{Student}(y_1), \mathsf{takesCourse}(y_1, y_2), \mathsf{Student}(y_3), \mathsf{takesCourse}(y_3, y_2), \mathsf{Course}(y_2),$ $\mathsf{advisor}(y_1, y_3), \mathsf{advisor}(y_3, y_4)$}
q_2 : {$\mathsf{headOf}(y_1, y_2), \mathsf{headOf}(y_3, y_2), \mathsf{Department}(y_2)$}
q_3 : {$\mathsf{Student}(y_1), \mathsf{takesCourse}(y_1, y_2), \mathsf{Course}(y_2), \mathsf{teacherOf}(y_2, y_3)$}
q_4 : {$\mathsf{Professor}(y_1), \mathsf{publicationAuthor}(y_2, y_1), \mathsf{Publication}(y_2), \mathsf{memberOf}(y_1, y_3),$ $\mathsf{Department}(y_3)$}
Uniprot queries:
q_1 : {$\mathsf{Protein}(y_1), \mathsf{annotation}(y_1, y_2), \mathsf{TransmembraneAnnotation}(y_2), \mathsf{range}(y_2, y_3)$}
q_2 : {$\mathsf{Protein}(y_1), \mathsf{organism}(y_1, y_2), \mathsf{annotation}(y_1, y_2)$}
q_3 : {$\mathsf{locatedIn}(y_1, y_2), \mathsf{cellularComponent}(y_2, y_3), \mathsf{cellularComponent}(y_4, y_3),$ $\mathsf{CellularComponent}(y_3)$}

Fig. 5: Queries used for proof of concept: all variables are existentially quantified

Proofs for the Main Technical Results

In the following, we will consider an RSA ontology $\mathcal{O}$ and a CQ $Q = \exists \vec{y}.\psi(\vec{x}, \vec{y})$. For $\mathcal{P}_{\mathcal{O},Q}$, $E_{\mathcal{O}}$, and $\pi(\mathcal{O})^{\approx,\top}$, we will refer to their LHMs as $\mathcal{M}$, $\mathcal{M}_c$ (*canonical*), and $\mathcal{M}_u$ (*universal*), respectively. Note that, as $\mathcal{P}_{\mathcal{O},Q}$ is stratified, it is the case that: $\mathcal{M}_c \subseteq \mathcal{M}$.

We start with some notations concerning terms and atoms. For terms s and t, we write $s \leq t$ ($s < t$) iff s is (strictly) contained in t. The root of a term t is its non-functional part: $root(f_1(f_2(\ldots(f_n(a))\ldots))) = a$. We say that a term t has type (A, S, C) if t is either of the form $v^{A,i}_{S,C}$ or of the form $f^{A}_{S,C}(v)$.

The derivation level of a ground atom $a = p(\vec{t}) \in M[P]$, where P is a stratified program, is denoted as $level(a, M[P])$ and is a pair of natural numbers (k, l) where k denotes the strata of p and l is the smallest number such that $a \in T^{l}_{\mathcal{P}_k}(U)$, where $U = \emptyset$, if $k = 1$, and $U = T^{\omega}_{\mathcal{P}_{k-1}}(U_i)$, otherwise. The derivation level of a ground term $t \in terms(M[P])$, where P is a stratified program, is denoted as $level(t, M[P])$ and is a pair of natural numbers (k, l) such that t occurs in an atom $a \in M[P]$ s.t. $level(a, M[P]) = (k, l)$, but t does not occur in any atom $a \in M[P]$ such that $level(a, M[P]) = (k', l')$, and $k' < k$, or $k' = k$ and $l' < l$. When the program P

has only one stratum, the stratum is dropped from the derivation level of corresponding atoms/terms.

We next relate terms in $\mathcal{M}_c$ and $\mathcal{M}_u$ to terms in M_{RSA}.

Lemma 1. *Let* $\eta_c : terms(\mathcal{M}_c) \to terms(M_{\mathsf{RSA}})$ *be the following function:* $\eta_c(t) = \begin{cases} \{a\}, \textit{if } t = a \in N_I \\ u^A_{R,B}, \textit{if } t \textit{ is of type } (A, R, B) \end{cases}$ *. Then, for every* $t_1, t_2 \in terms(\mathcal{M}_c)$ *it holds that:*

- $A(t_1) \in \mathcal{M}_c$ *implies* $A(\eta_c(t_1)) \in M_{\mathsf{RSA}}$,
- $R(t_1, t_2) \in \mathcal{M}_c$ *implies* $R(\eta_c(t_1), \eta_c(t_2)) \in M_{\mathsf{RSA}}$,
- $t_1 \approx t_2 \in \mathcal{M}_c$ *implies* $\eta_c(t_1) \approx \eta_c(t_2) \in M_{\mathsf{RSA}}$.

Proof. By induction on the derivation level of atoms in $\mathcal{M}_c$. $\square$

Lemma 2. *Let* $\eta_u : terms(\mathcal{M}_u) \to terms(M_{\mathsf{RSA}})$ *be the following function:* $\eta_u(t) = \begin{cases} \{a\}, \textit{if } t = a \in N_I \\ u^A_{R,B}, \textit{if } t \textit{ is of type } (A, R, B) \end{cases}$ *. Then, for every* $t_1, t_2 \in terms(\mathcal{M}_u)$ *it holds that:*

- $A(t_1) \in \mathcal{M}_u$ *implies* $A(\eta_u(t_1)) \in M_{\mathsf{RSA}}$,
- $R(t_1, t_2) \in \mathcal{M}_u$ *implies* $R(\eta_u(t_1), \eta_u(t_2)) \in M_{\mathsf{RSA}}$,
- $t_1 \approx t_2 \in \mathcal{M}_u$ *implies* $\eta_u(t_1) \approx \eta_u(t_2) \in M_{\mathsf{RSA}}$.

Proof. By induction on the derivation level of atoms in $\mathcal{M}_u$. $\square$

The previous lemmas will prove useful to characterize terms in $\mathcal{M}_c$ (resp. $\mathcal{M}_u$):

Lemma 3. *Let* $t_1, t_2 \in terms(\mathcal{M}_c)$*. Then,* $t_1 \approx t_2 \in \mathcal{M}_c$ *implies one of the following:*

1. $t_1 \approx a$*, for some* $a \in N_I$*,*
2. t_1 *is of the form* $v^{A,i}_{R,B}$ *and* t_1 *and* t_2 *are identical (the same term), or*
3. t_1 *is of the form* $f(u)$*, and* t_2 *is of the form* $g(v)$*, with* $u \approx v \in \mathcal{M}_c$*.*

Proof.

We show the claim of the lemma together with the following additional claims by induction on the derivation level of atoms in $\mathcal{M}_c$:

i) $R(t_1, t_2) \in \mathcal{M}_c$, there exists a role S such that $R \sqsubseteq^*_{\mathcal{R}} S$ and S occurs in an axiom (T4), and a term $t_3 \in terms(\mathcal{M}_c)$ s.t. $t_1 \approx t_3 \in \mathcal{M}_c$ with $\eta(c_1) \neq \eta(c_3)$, implies that $t_2 \approx f(t_1) \in \mathcal{M}_c$ for some function symbol f occurring in $\mathcal{M}_c$ and either $t_2 \approx a$, for some $a \in N_{\mathsf{I}}$ or t_2 is of the form $g(u)$ with $u \approx t_1 \in \mathcal{M}_c$.

ii) $R(t_1, t_2) \in \mathcal{M}_c$, there exists a role S such that $R \sqsubseteq^*_{\mathcal{R}} \mathsf{Inv}(S)$ and S occurs in an axiom (T4), and a term $t_3 \in terms(\mathcal{M}_c)$ s.t. $t_1 \approx t_3 \in \mathcal{M}_c$ with $\eta(c_1) \neq \eta(c_3)$, implies that $t_1 \approx f(t_2) \in \mathcal{M}_c$ for some function symbol f occurring in $\mathcal{M}_c$ and either $t_1 \approx a$, for some $a \in N_{\mathsf{I}}$ or t_1 is of the form $g(u)$ with $u \approx t_2 \in \mathcal{M}_c$.

In the following let a be an atom in $\mathcal{M}_c$. We distinguish between:

i) $a = R(t_1, t_2)$, there exists a role S such that $R \sqsubseteq^*_{\mathcal{R}} S$ and S occurs in an axiom (T4), and a term $t_3 \in terms(\mathcal{M}_c)$ s.t. $t_1 \approx t_3 \in \mathcal{M}_c$ with $\eta(c_1) \neq \eta(c_3)$. Then, there must be some rule in E_O:

1. $C(x) \rightarrow R(x, f^C_{R,D}(x)) \wedge D(f^C_{R,D}(x))$ such that: $C(t_1) \in \mathcal{M}_c$ and $t_2 = f^C_{R,D}(t_1)$ - claim i) is fulfilled.
2. $C(x) \rightarrow R(x, v^C_{R,D}) \wedge D(v^C_{R,D})$ - contradiction with the fact that R is unsafe.
3. $T(x, y) \rightarrow R(x, y)$ such that $T(t_1, t_2) \in \mathcal{M}_c$ and $level(T(t_1, t_2), \mathcal{M}_c) < level(R(t_1, t_2), \mathcal{M}_c)$. Then T has all the properties of R: claim i) follows from the IH.
4. $\mathsf{Inv}(R)(x, y) \rightarrow R(x, y)$ such that $\mathsf{Inv}(R)(t_2, t_1) \in \mathcal{M}_c$ and $level(\mathsf{Inv}(R)(t_1, t_2), \mathcal{M}_c) < level(R(t_1, t_2), \mathcal{M}_c)$. Then $\mathsf{Inv}(R)$ fulfils all the conditions for claim ii): from the IH, it follows that $t_2 \approx f(t_1)$ and either $t_2 \approx a$, for some $a \in N_\mathsf{I}$ or t_2 is of the form $g(u)$ with $u \approx t_1 \in \mathcal{M}_c$.
5. $R(x, y) \wedge y \approx z \rightarrow R(x, z)$ and a term t_3 such that $R(t_1, t_3), t_3 \approx t_2 \in \mathcal{M}_c$. From the IH: $t_3 \approx f(t_1)$ and either $t_3 \approx a$, for some $a \in N_\mathsf{I}$ or t_3 is of the form $g(u)$ with $u \approx t_1 \in \mathcal{M}_c$. Then, $t_2 \approx f(t_1)$ and either $t_2 \approx a$, for some $a \in N_\mathsf{I}$, or t_3 is of the form $g(u)$, with $u \approx t_1 \in \mathcal{M}_c$ and t_2 is of the form $h(w)$ with $u \approx w \in \mathcal{M}_c$. But then, $w \approx t_1 \in \mathcal{M}_c$.
6. $R(x, y) \wedge x \approx z \rightarrow R(z, y)$ and a term t_3 such that $R(t_3, t_2), t_3 \approx t_1 \in \mathcal{M}_c$. From the IH: $t_2 \approx f(t_3)$ and either $t_2 \approx a$, for some $a \in N_\mathsf{I}$ or t_2 is of the form $g(u)$ with $u \approx t_3 \in \mathcal{M}_c$. Then, $t_2 \approx f(t_1)$ and either $t_2 \approx a$, for some $a \in N_\mathsf{I}$ or t_2 is of the form $g(u)$ with $u \approx t_1 \in \mathcal{M}_c$.

ii) $a = R(t_1, t_2)$, there exists a role S such that $R \sqsubseteq^*_\mathcal{R} \mathsf{Inv}(S)$ and S occurs in an axiom (T4), and a term $t_3 \in terms(\mathcal{M}_c)$ s.t. $t_1 \approx t_3 \in \mathcal{M}_c$ with $\eta(c_1) \neq \eta(c_3)$. Then, there must be some rule in E_O:

1. $C(x) \rightarrow R(x, f^C_{R,D}(x)) \wedge D(f^C_{R,D}(x))$ such that: $C(t_1) \in \mathcal{M}_c$ and $t_2 = f^C_{R,D}(t_1)$. Then, from Lemma 1 it follows that: $R(\eta_c(t_1), u^C_{D,R}) \in M_{\mathsf{RSA}}$. But then, $\mathcal{O}$ is not equality-safe – contradiction.
2. $C(x) \rightarrow R(x, v^C_{R,D}) \wedge D(v^C_{R,D})$ - contradiction with the fact that R is unsafe.
3. $T(x, y) \rightarrow R(x, y)$ such that $T(t_1, t_2) \in \mathcal{M}_c$: similar to case i) 3. above.
4. $\mathsf{Inv}(R)(x, y) \rightarrow R(x, y)$ such that $\mathsf{Inv}(R)(t_2, t_1) \in \mathcal{M}_c$: similar to case i) 4. above.
5. $R(x, y) \wedge y \approx z \rightarrow R(x, z)$ and a term t_3 such that $R(t_1, t_3), t_3 \approx t_2 \in \mathcal{M}_c$: similar to case i) 5. above.
6. $R(x, y) \wedge x \approx z \rightarrow R(z, y)$ and a term t_3 such that $R(t_3, t_2), t_3 \approx t_1 \in \mathcal{M}_c$: similar to case i) 6. above.

iii) $a = t_1 \approx t_2$. Then, there must be some rule in E_O:

1. $A(x) \rightarrow x \approx a$ such that $A(t_1) \in \mathcal{M}_c$ and $t_2 = a$: condition 1. of the lemma is fulfilled;
2. $\top(x) \rightarrow x \approx x$ such that $t_1 = t_2 = x$: condition 2. or 3. of the lemma holds;
3. $x \approx y \rightarrow y \approx x$ such that: $t_2 \approx t_1$: some condition of the lemma is fulfilled (as all conditions are symmetric as concerns t_1 and t_2)
4. $x \approx y \wedge y \approx z \rightarrow x \approx z$ and a term t_3 such that $t_1 \approx t_3, t_3 \approx t_2 \in \mathcal{M}_c$. From the IH, one of the following holds:
   - $t_1 \approx a \in \mathcal{M}_c$, for some $a \in N_\mathsf{I}$. Then, $t_3 \approx a \in \mathcal{M}_c$, as well.
   - t_1 and t_2 are identical. Then, whatever condition of the lemma holds w.r.t t_3 and t_2 will hold also w.r.t. t_1 and t_2.

- t_1 is of the form $f(u)$, t_3 is of the form $g(v)$, and t_2 is of the form $h(w)$ with $u \approx v \in \mathcal{M}_c$ and $v \approx w \in \mathcal{M}_c$. Then, $u \approx w \in \mathcal{M}_c$ and claim 3. of the lemma holds for t_1 and t_2.

5. $A(x) \wedge S(x,y) \wedge B(y) \wedge S(x,z) \wedge B(z) \rightarrow y \approx z$ and a term t_3 such that $A(t_3), S(t_3,t_2), B(t_2), S(t_3,t_1), B(t_1) \in \mathcal{M}_c$. We distinguish between:
   - $\eta(t_1) = \eta(t_2)$: then, either $t_1 = t_2$–in which case, the claim of the lemma trivially holds, or $t_1 \neq t_2$, but t_1 and t_2 have the same type (C, R, D)–in which case $\mathcal{O}$ is not RSA – contradiction.
   - $\eta(t_1) \neq \eta(t_2)$: then, from claim i) above it follows that $t_2 \approx f(t_3) \in \mathcal{M}_c$ and $t_1 \approx g(t_3) \in \mathcal{M}_c$ and either:
     - $t_1 \approx a \in \mathcal{M}_c$, for some $a \in N_\mathsf{I}$ (in which case $t_2 \approx a \in \mathcal{M}_c$, as well): then claim 1. of the lemma holds, or
     - $t_1 = h(u)$, with $u \approx t_3 \in \mathcal{M}_c$, and $t_2 = i(w)$, with $w \approx t_3 \in \mathcal{M}_c$. Then, $u \approx w \in \mathcal{M}_c$ and claim 3. of the lemma holds.

Lemma 4. *Let $t_1, t_2 \in terms(\mathcal{M}_u)$. Then $t_1 \approx t_2 \in \mathcal{M}_u$ implies that either:*

1. *$t_1 \approx a \in \mathcal{M}_u$, for some $a \in N_\mathsf{I}$, or*
2. *t_1 is of the form $f(u)$ and t_2 is of the form $g(v)$ with $u \approx v \in \mathcal{M}_u$.*

Proof. Similar to the proof for Lemma 3 using Lemma 2. □

We next establish some relationships between the canonical model $\mathcal{M}_c$ and the universal model $\mathcal{M}_u$.

Definition 6. *A role R in $\mathcal{O}$ is said to be* forward-sound *if for each axiom of type $A \sqsubseteq \exists S.B$ in $\mathcal{O}$ with S being a safe role: $S \not\sqsubseteq^*_\mathcal{R} R$. If for every axiom of the same type, $S \not\sqsubseteq^*_\mathcal{R} \mathsf{Inv}(R)$, S is said to be* backward-sound.

Definition 7. *Let $\mu : terms(\mathcal{M}_c) \rightarrow 2^{terms(\mathcal{M}_u)}$ be the following function:*

$$\mu(t) = \begin{cases} \{t\}, & \text{if } t \in N_\mathsf{I} \\ \{f^A_{R,B}(v) \mid v \in \mu(u)\}, & \text{if } t = f^A_{R,B}(u) \\ \{f^A_{R,B}(x) \mid f^A_{R,B}(x) \in terms(\mathcal{M}_u)\} & \text{if } t = v^{A,i}_{R,B} \end{cases}$$

Lemma 5. *Let μ be as in Definition 7. Then:*

i) *for every $t \in terms(\mathcal{M}_c)$, $\mu(t) \neq \emptyset$,*
ii) *$A(t) \in \mathcal{M}_c$ implies $A(u) \in \mathcal{M}_u$, for every $u \in \mu(t)$,*
iii) *$R^f(t_1,t_2) \in \mathcal{M}_c \wedge t_2 \notin N_\mathsf{I}$ implies $R(u, f^A_{S,C}(u)) \in \mathcal{M}_u$ and $f^A_{S,C}(u) \approx v \in \mathcal{M}_u$, with $v \in \mu(t_2)$, for every $u \in \mu(t_1)$, where t_2 is of type (A, S, C),*
iv) *$R^f(t_1,t_2) \in \mathcal{M}_c \wedge t_2 \in N_\mathsf{I}$ implies $R(u,t_2) \in \mathcal{M}_u$, for every $u \in \mu(t_1)$,*
v) *$R^b(t_1,t_2) \in \mathcal{M}_c \wedge t_1 \notin N_\mathsf{I}$ implies $R(f^A_{S,C}(u), u) \in \mathcal{M}_u$ and $f^A_{S,C}(u) \approx v \in \mathcal{M}_u$, with $v \in \mu(t_1)$, for every $u \in \mu(t_2)$, where t_1 is of type (A, S, C),*
vi) *$R^b(t_1,t_2) \in \mathcal{M}_c \wedge t_1 \in N_\mathsf{I}$ implies $R(t_1,u) \in \mathcal{M}_u$, for every $u \in \mu(t_2)$,*
vii) *$R(t_1,t_2) \in \mathcal{M}_c \wedge NI(t_1) \in \mathcal{M}_c \wedge NI(t_2) \in \mathcal{M}_c$ implies $R(\sigma(t_1), \sigma(t_2)) \in \mathcal{M}_u$*

viii) *$t_1 \approx t_2 \in \mathcal{M}_c$ implies for every $u_1 \in \mu(t_1)$, there exists $u_2 \in \mu(t_2)$ s.t. $u_1 \approx u_2 \in \mathcal{M}_u$, and for every $u_2 \in \mu(t_2)$, there exists $u_1 \in \mu(t_1)$ s.t. $u_1 \approx u_2 \in \mathcal{M}_u$,*

ix) *$R(t_1, t_2) \in \mathcal{M}_c$, with R being forward-sound, implies for every $v \in \mu(t_2)$ there exists $u \in \mu(t_1)$ such that $R(u, v) \in \mathcal{M}_u$,*

x) *$R(t_1, t_2) \in \mathcal{M}_c$, with R being backward-sound, implies for every $u \in \mu(t_1)$ there exists $v \in \mu(t_2)$ such that $R(u, v) \in \mathcal{M}_u$.*

Proof. By induction on the derivation level of atoms/terms in $\mathcal{M}_c$.

IB: the hypothesis holds for every ABox assertion and named individual.

IH: the hypothesis holds for every atom/term a with $level(a, \mathcal{M}_c) < k$, for some $k > 1$. We show that it also holds for every atom/term with $level(a, \mathcal{M}_c) = k$.

i) $t \in terms(\mathcal{M}_c)$, $t \notin N_\mathsf{I}$. Then t has one of the forms:

1. $v^{A,i}_{R,B}$: then, it has been introduced in $\mathcal{M}_c$ via a rule $A(x) \to R(x, v^{A,i}_{R,B}) \wedge B(v^{A,i}_{R,B})$, where $x = t'$, for some $t' \in terms(\mathcal{M}_c)$, and $\pi(\mathcal{O})^{\approx,\top}$ contains a counterpart rule $A(x) \to R(x, f^A_{R,B}(x)) \wedge B(f^A_{R,B}(x))$. From the IH, $\mu(t') \neq \emptyset$ and $A(u) \in \mathcal{M}_u$, for every $u \in \mu(t')$. Thus, $R(u, f^A_{R,B}(u)) \in \mathcal{M}_u$. But $f^A_{R,B}(u) \in \mu(v^{A,i}_{R,B})$, and thus $\mu(a) \neq \emptyset$.
2. $f^A_{R,B}(t')$. From the IH: $\mu(t') \neq \emptyset$, thus $\mu(f^A_{R,B}(t)) \neq \emptyset$.

ii) $a = A(t)$. Then, there must be a rule in $E_\mathcal{O}$:

1. $A_1(x) \wedge \ldots \wedge A_n(x) \to A(x)$ such that $A_i(t) \in \mathcal{M}_c$. From the IH: $\mu(t) \neq \emptyset$ and $A_i(u) \in \mathcal{M}_u$ for every $u \in \mu(t)$. Thus, $A(u) \in \mathcal{M}_u$ for every $u \in \mu(t)$.
2. $B(x) \to R(x, f^B_{R,A}(x)), A(f^B_{R,A}(x))$ and some term $t' \in \mathcal{M}_c$ s.t. $B(t') \in \mathcal{M}_c$ and $t = f^B_{R,A}(t')$. Then, $B(u') \in \mathcal{M}_u$, for every $u' \in \mu(t')$, and thus $A(f^B_{R,A}(u')) \in \mathcal{M}_u$ for every $u' \in \mu(t')$, or for every $u \in \mu(f^B_{R,A}(t'))$: $A(u \in \mathcal{M}_u)$.
3. $B(x) \to R(x, v^B_{R,A}), A(v^B_{R,A})$ and some term $t' \in \mathcal{M}_c$ s.t. $B(t') \in \mathcal{M}_c$ and $t = v^B_{R,A}$: similar as above.
4. $R(x, y) \wedge B(y) \to A(x)$, and some term t' such that $R(t, t'), B(t') \in \mathcal{M}_c$. We note that as R occurs on the l.h.s. of an axiom it must be a backward-sound role. Thus, for every $u \in \mu(t)$, there exists $v \in \mu(t')$ such that $R(u, v) \in \mathcal{M}_u$. Then, $B(t')$ implies $B(v)$ and for every $u \in \mu(t)$, $A(u) \in \mathcal{M}_u$.
5. $A(x) \wedge x \approx y \to A(y)$, and some terms t, t' such that $A(t'), t' \approx t \in \mathcal{M}_c$. Then, for every $u \in \mu(t)$, there exists $v \in \mu(t')$ such that $v \approx u \in \mathcal{M}_u$. But, then $A(v) \in \mathcal{M}_u$ and thus for every $u \in \mu(t)$, $A(u) \in \mathcal{M}_u$.

iii) $a = R^f(t_1, t_2)$ and $NI(t_2) \notin \mathcal{M}_c$. Then there must be a rule in $E_\mathcal{O}$:

1. $A(x) \to R^f(x, v^{A,i}_{R,B}), B(v^{A,i}_{R,B})$ such that $A(t_1) \in \mathcal{M}_c$ and $t_2 = v^{A,i}_{R,B}$. Then, t_2 is of type (A, R, B) and for every $u \in \mu(t_1)$, $A(u) \in \mathcal{M}_u$, and there exists a rule $A(x) \to R(x, f^A_{R,B}(x)), B(f^A_{R,B}(x))$ in $\pi(\mathcal{O})^{\approx,\top}$. Thus, $R(u, f^A_{R,B}(u)) \in \mathcal{M}_u$, for every $u \in \mu(t_1)$, and obviously, $f^A_{R,B}(u) \approx f^A_{R,B}(u) \in \mathcal{M}_u$ and $f^A_{R,B}(u) \in \mu(t_2)$.
2. $A(x) \to R^f(x, f^A_{R,B}(x)), B(f^A_{R,B}(x))$ such that $A(t_1) \in \mathcal{M}_c$ and $t_2 = f^A_{R,B}(x)$. Similar to the previous case.

3. $S^f(x,y) \rightarrow R^f(x,y)$ such that $S^f(t_1,t_2) \in \mathcal{M}_c$. From the IH: $S(u, f^A_{S,C}(u)) \in \mathcal{M}_u$ and $f^A_{S,C}(u) \approx v \in \mathcal{M}_u$ and $v \in \mu(t_2)$, for every $u \in \mu(t_1)$, where t_2 is of type (A,S,C), thus $R(u, f^A_{S,C}(u)) \in \mathcal{M}_u$ and $f^A_{S,C}(u) \approx v \in \mathcal{M}_u$ and $v \in \mu(t_2)$, for every $u \in \mu(t_1)$.
4. $\mathsf{Inv}(R)^b(x,y) \rightarrow R^f(y,x)$ such that $\mathsf{Inv}(R)^b(t_2,t_1) \in \mathcal{M}_c$. From the IH: $\mathsf{Inv}(R)(f^A_{S,C}(u), u) \in \mathcal{M}_u$ and $f^A_{S,C}(u) \approx v \in \mathcal{M}_u$ and $v \in \mu(t_2)$, for every $u \in \mu(t_1)$, where t_2 is of type (A,S,C), thus $R(u, f^A_{S,C}(u)) \in \mathcal{M}_u$ and $f^A_{S,C}(u) \approx v \in \mathcal{M}_u$ and $v \in \mu(t_2)$, for every $u \in \mu(t_1)$.
5. $R^f(x,y), y \approx z \rightarrow R^f(x,z)$ and some term t_3 such that $R^f(t_1,t_3), t_3 \approx t_2 \in \mathcal{M}_c$. If $t_2 = v^{A,i}_{S,C}$, then $t_3 = v^{A,i}_{S,C}$, as well (Lemma 3), and thus $R^f(t_1,t_3) = R^f(t_1,t_2)$. In this case, the IH cannot be applied as $level(\ R^f\ (\ t_1,t_3), \mathcal{M}_c) = level(R^f(t_1,t_2), \mathcal{M}_c)$. Otherwise, $t_2 = f^A_{S,C}(s)$. Assume then, that t_3 has type (B,T,D), and thus $t_3 = f^B_{T,D}(w)$.

   From the IH we have that for every $u \in \mu(t_1)$, $R(u, f^B_{T,D}(u)) \in \mathcal{M}_u$ (1) and $f^B_{T,D}(u) \in \mu(t_3)$. Furthermore, for $f^B_{T,D}(u) \in \mu(t_3)$ there must be some $t \in \mu(t_2)$ such that $f^B_{T,D}(u) \approx t \in \mathcal{M}_u$. As $t \in \mu(t_2)$, it follows that $t = f^A_{S,C}(v')$, where $v' \in \mu(v)$, and thus $f^B_{T,D}(u) \approx f^A_{S,C}(v') \in \mathcal{M}_u$. From Lemma 3 it follows that $u \approx v' \in \mathcal{M}_u$, and thus $f^B_{T,D}(u) \approx f^A_{S,C}(u) \in \mathcal{M}_u$ (2). Finally, from (1) and (2), it follows that $R(u, f^A_{S,C}(u)) \in \mathcal{M}_u$. Furthermore, $f^A_{S,C}(u) \approx f^A_{S,C}(v') \in \mathcal{M}_u$ and $f^A_{S,C}(v') \in \mu(t_2)$.
6. $R^f(x,y), x \approx z \rightarrow R^f(z,y)$, with $R^f(t_3,t_2) \in \mathcal{M}_c$ and $t_3 \approx t_1 \in \mathcal{M}_c$. Then, from the IH, for every $u \in \mu(t_1)$, there must be some $v \in \mu(t_3)$ such that $u \approx v \in \mathcal{M}_u$, and for every $v \in \mu(t_3)$: $R(v, f^A_{S,C}(v)) \in \mathcal{M}_u$, $f^A_{S,C}(v) \approx w \in \mathcal{M}_u$, and $w \in \mu(t_2)$. Then, for every $u \in \mu(t_1)$, $R(u, f^A_{S,C}(u)) \in \mathcal{M}_u$, $f^A_{S,C}(u) \approx w \in \mathcal{M}_u$, and $w \in \mu(t_2)$.

iv) $a = R^f(t_1,t_2) \in \mathcal{M}_c$ and $NI(t_2) \in \mathcal{M}_c$.
Then, there must be a rule in $E_{\mathcal{O}}$:
1. $S^f(x,y) \rightarrow R^f(x,y)$ such that $S^f(t_1,t_2) \in \mathcal{M}_c$ and $NI(t_2) \in \mathcal{M}_c$. From the IH: $S(u, \sigma(t_2)) \in \mathcal{M}_u$, for every $u \in \mu(t_1)$, thus $R(u, \sigma(t_2)) \in \mathcal{M}_u$, for every $u \in \mu(t_1)$.
2. $\mathsf{Inv}(R)^b(x,y) \rightarrow R^f(y,x)$ such that $\mathsf{Inv}(R)^b(t_2,t_1) \in \mathcal{M}_c$ and $NI(t_2) \in \mathcal{M}_c$. From the IH: $\mathsf{Inv}(R)(\sigma(t_2), u) \in \mathcal{M}_u$, for every $u \in \mu(t_1)$, thus $R(u, \sigma(t_2)) \in \mathcal{M}_u$, for every $u \in \mu(t_1)$.
3. $R^f(x,y), y \approx z \rightarrow R^f(x,z)$ and some term t_3 such that $R^f(t_1,t_3), t_3 \approx t_2, NI(t_2) \in \mathcal{M}_c$. Then $NI(t_3) \in \mathcal{M}_c$ and from the IH: for every $u \in \mu(t_1)$, $R(u, \sigma(t_3)) = R(u, \sigma(t_2)) \in \mathcal{M}_u$.
4. $R^f(x,y), x \approx z \rightarrow R^f(z,y)$, with $R^f(t_3,t_2) \in \mathcal{M}_c$, $\sigma(t_2) \in \mathcal{M}_c$ and $t_3 \approx t_1 \in \mathcal{M}_c$. Then, from the IH, for every $u \in \mu(t_1)$, there must be some $v \in \mu(t_3)$ such that $u \approx v \in \mathcal{M}_u$, and for every $v \in \mu(t_3)$: $R(v, \sigma(t_2)) \in \mathcal{M}_u$. Then, for every $u \in \mu(t_1)$, $R(u, \sigma(t_2)) \in \mathcal{M}_u$.

v) $R^b(t_1,t_2) \in \mathcal{M}_c$ and $NI(t_1) \notin \mathcal{M}_c$. Similar to case iii) above.
vi) $R^b(t_1,t_2) \in \mathcal{M}_c$ and $NI(t_1) \in \mathcal{M}_c$. Similar to case iv) above.
vii) $R(t_1,t_2) \in \mathcal{M}_c$ and $NI(t_1) \in \mathcal{M}_c \wedge NI(t_2) \in \mathcal{M}_c$. Similar to case iii) above.

viii) $t_1 \approx t_2 \in \mathcal{M}_c$. Then, there must be a rule in $E_{\mathcal{O}}$:

1. $A(x) \wedge S(x,y) \wedge B(y) \wedge S(x,z) \wedge B(z) \rightarrow y \approx z$ and a term $t_3 \in terms(\mathcal{M}_c)$ such that $A(t_3), S(t_3,t_1), B(t_1), S(t_3,t_2), B(t_2), \in \mathcal{M}_c$. Then, S is both a forward-sound and a backward-sound role.
   From the IH, for every $u_1 \in \mu(t_1)$, $B(t_1) \in \mathcal{M}_u$, and there must be some $u_3 \in \mu(t_3)$ such that $S(u_3,u_1) \in \mathcal{M}_u$. Then, $A(u_3) \in \mathcal{M}_u$, and there must be some $u_2 \in \mu(t_2)$ s.t. $S(u_3,u_2) \in \mathcal{M}_u$ and $B(u_2) \in \mathcal{M}_u$. Then, by applying the counterpart equality rule in $\pi(\mathcal{O})^{\approx,\top}$ we obtain: $u_1 \approx u_2 \in \mathcal{M}_u$.
   It can be shown similarly to above, that for every $u_2 \in \mu(t_2)$, there exists $u_1 \in \mu(t_1)$ such that $u_1 \approx u_2 \in \mathcal{M}_u$.
2. $A(x) \rightarrow x \approx a$, with $A(t_1) \in \mathcal{M}_c$ and $t_2 = a$. From the IH, for every $u \in \mu(t_1)$, $A(u) \in \mathcal{M}_u$, and thus $u \approx a \in \mathcal{M}_u$. Conversely, $\mu(a) = \{a\}$, and $\mu(t_1) \neq \emptyset$, thus for every $t_2 \in \mu(a)$, there exists $u \in \mu(t_1)$ s.t. $u \approx t_2 \in umodel$.
3. $x \approx y \rightarrow y \approx x$: follows from the symmetry of the IH.
4. $x \approx y \wedge y \approx z \rightarrow x \approx z$: follows from the IH, similar to case 1. above.

ix) $R(t_1,t_2) \in \mathcal{M}_c$, with R being forward-sound. Then, there must be a rule in $E_{\mathcal{O}}$:

1. $A(x) \rightarrow R^f(x, f^A_{R,B}(x)), B(f^A_{R,B}(x))$ such that $A(t_1) \in \mathcal{M}_c$ and $t_2 = f^A_{R,B}(t_1)$. Then, for every $u \in \mu(t_1)$, $A(u) \in \mathcal{M}_u$, and there exists a rule $A(x) \rightarrow R(x, f^A_{R,B}(x)), B(f^A_{R,B}(x))$ in $\pi(\mathcal{O})^{\approx,\top}$. Thus, $R(u, f^A_{R,B}(u)) \in \mathcal{M}_u$, for every $f^A_{R,B}(u) \in \mu(t_2)$.
2. $A(x) \rightarrow R^f(x, v^{A,i}_{R,B}), B(v^{A,i}_{R,B})$ such that $A(t_1) \in \mathcal{M}_c$ and $t_2 = v^A_{R,B}$. Then, R must be safe – contradiction with R being forward-sound.
3. $S(x,y) \rightarrow R(x,y)$ and $S(t_1,t_2) \in \mathcal{M}_c$: then S must be forward-sound as well and the claim follows from the IH.
4. $\mathsf{Inv}(R)(x,y) \rightarrow R(y,x)$ and $\mathsf{Inv}(R)(t_2,t_1) \in \mathcal{M}_c$: then $\mathsf{Inv}(R)$ is backward-sound and the claim follows from the IH.
5. $R(x,y), y \approx z \rightarrow R(x,z)$ and some term t_3 such that $R(t_1,t_3), t_3 \approx t_2 \in \mathcal{M}_c$. From the IH we have that for every $u_2 \in \mu(t_2)$, there exists $u_3 \in \mu(t_3)$ such that $u_2 \approx u_3 \in \mathcal{M}_c$. Further on, as R is forward-sound, for every $u_3 \in \mu(t_3)$, there must be some $u_1 \in \mu(t_1)$ such that $R(u_1,u_3) \in \mathcal{M}_c$. Then, by applying the counterpart rule in $\pi(\mathcal{O})^{\approx,\top}$ we obtain that $R(u_1,u_2) \in \mathcal{M}_u$, for every $u_2 \in \mu(t_2)$.
6. $R(x,y), x \approx z \rightarrow R(z,y)$, with $R(t_3,t_2) \in \mathcal{M}_c$ and $t_3 \approx t_1 \in \mathcal{M}_c$. Similar to above.

x) $R(t_1,t_2) \in \mathcal{M}_c$, with R being backward-sound: similar to case ix) above taking into account that the inverse of a backward-sound role is a forward-sound role.

Definition 8. *Let Φ be a conjunction of atoms of the form:*

$$\bigwedge_{i=1}^{m} A_i(t_i) \wedge \bigwedge_{j=1}^{n} R_j(u_{1j}, u_{2j}).$$

An adornment for Φ is a vector $\vec{a}$ such that $|\vec{a}| = n$, and $a_j \in \{f, b, \text{\textvisiblespace}\}$, for every $1 \leq j \leq n$ (where $\text{\textvisiblespace}$ denotes the empty adorning: $R^{\text{\textvisiblespace}}$ is the same as R).

Then, we denote with $\Phi^{\vec{a}}$ the adorned formula:

$$\bigwedge_{i=1}^{m} A_i(t_i) \wedge \bigwedge_{j=1}^{n} R_j^{a_j}(u_{1j}, u_{2j}).$$

Definition 9. *Let $\Phi^{\vec{a}}$ be an adorned formula of the form:*

$$\bigwedge_{i=1}^{m} A_i(t_i) \wedge \bigwedge_{j=1}^{n} R_j^{a_j}(u_{1j}, u_{2j}).$$

Then, the normal form of $\Phi^{\vec{a}}$, denoted $\Phi_n^{\vec{a}}$, is the formula:

$$\bigwedge_{i=1}^{m} A_i(t_i) \wedge \bigwedge_{j=1}^{n} L_j$$

where:

$$L_j = \begin{cases} R(u_{1j}, u_{2j}), & \text{if } a_j = \textvisiblespace \\ R^f(u_{1j}, u_{2j}), & \text{if } a_j = f \\ \mathsf{Inv}(R)^f(u_{2j}, u_{1j}), & \text{if } a_j = b. \end{cases}$$

Lemma 6. *Let $\vec{a}$ be an adornment for $\psi(\vec{x}, \vec{y})$ and let $\lambda : terms(Q) \to terms(\mathcal{M})$ be a homomorphism. Then: $M \models (\psi(\lambda(\vec{x}), \lambda(\vec{y})))^{\vec{a}}$ iff $M \models (\psi(\lambda(\vec{x}), \lambda(\vec{y})))_n^{\vec{a}}$.*

Definition 10. *Let $\lambda : terms(Q) \to terms(\mathcal{M})$ be a homomorphism and let $\vec{a}$ be an adornment for $\psi(\vec{x}, \vec{y})$. Then, $(\lambda, \vec{a})$ is said to be an* adorned match *for Q over $\mathcal{M}$ iff the following hold:*

1. *$\mathcal{M} \models (\psi(\lambda(\vec{x}), \lambda(\vec{y})))^{\vec{a}}$, and*
2. *$R(t_1, t_2) \in (\psi(\lambda(\vec{x}), \lambda(\vec{y})))^{\vec{a}}$ implies $R^f(t_1, t_2) \notin \mathcal{M}$ and $R^b(t_1, t_2) \notin \mathcal{M}$.*

When the adornment $\vec{a}$ is irrelevant/not applicable (i.e. $\mathcal{M} \models \psi(\lambda(\vec{x}), \lambda(\vec{y}))$) we say that λ is a match *for Q over $\mathcal{M}$.*

Definition 11. *Let $(\lambda, \vec{a})$ be an adorned match for Q w.r.t. $\mathcal{M}$. We say that $(\lambda, \vec{a})$ is* non-anonymous *if $named(\lambda(x)) \in \mathcal{M}$, for every $x \in \vec{x}$.*

Definition 12. *Let $(\lambda, \vec{a})$ be an adorned match for Q w.r.t. $\mathcal{M}$. We say that $(\lambda, \vec{a})$ is* fork-free *iff for every two atoms of the form $R^f(s, y_i)$, $S^f(t, y_j) \in (\psi(\vec{x}, \vec{y}))_n^{\vec{a}}$, such that $s, t \in terms(Q)$, y_i, $y_j \in \vec{y}$, and $\mathsf{id}(\lambda(\vec{x}), \lambda(\vec{y}), i, j) \in \mathcal{M}$, it is the case that $\lambda(s) \approx \lambda(t)$.*

Definition 13. *Let $(\lambda, \vec{a})$ be an adorned match for Q w.r.t. $\mathcal{M}$. We say that $(\lambda, \vec{a})$ is* acyclic *iff there is no sequence of atoms:*

$$R_{o_1}^f(y_{l_1}, y_{l_2}), R_{o_2}^f(y_{l_3}, y_{l_4}), \ldots, R_{o_p}^f(y_{l_{2p-1}}, y_{l_{2p}}) \in (\psi(\vec{x}, \vec{y}))_n^{\vec{a}}$$

such that:

1. $\mathsf{id}(\lambda(\vec{x}), \lambda(\vec{y}), l_{2i}, l_{2i+1}) \in \mathcal{M}$, *for every* $1 \leq i \leq p$ *(*$l_{2p+1} = l_1$*), and*
2. $NI(\lambda(y_{l_j})) \notin \mathcal{M}$, *for every* $1 \leq j \leq 2p$.

Lemma 7. *For a given substitution* $\lambda : \vec{x} \to terms(\mathcal{M})$, *it is the case that* $\mathcal{M} \models ANS(\lambda(x))$ *iff there exists an adorned match* $(\lambda', \vec{a})$ *for* Q *over* $\mathcal{M}$ *which is non-anonymous, fork-free, and acyclic, where* λ' *is a homomorphism that extends* λ *to* $terms(Q)$.

Proof. From the semantics of $\pi(\mathcal{O})^{\approx,\top}$ and Lemma 6. □

Definition 14. *Let* $(\lambda, \vec{a})$ *be an adorned match for* Q *over* $\mathcal{M}_c$ *and let* $id_{(\lambda,\vec{a})} : \vec{y} \times \vec{y}$ *be the binary relationship containing exactly the pairs* (y_i, y_j) *for which* $\mathsf{id}(\lambda(\vec{x}), \lambda(\vec{y}), i, j) \in \mathcal{M}_c$.

Claim. For any given adorned match $(\lambda, \vec{a})$ for Q over $\mathcal{M}$, $id_{(\lambda,\vec{a})}$ is a congruence relationship.

Definition 15. *For* $(\lambda, \vec{a})$ *an adorned match for* Q *over* $\mathcal{M}_c$, *let* $\tau : terms(Q) \to terms(Q)$ *be such that* $\tau(y)$, *where* $y \in \vec{y}$, *maps* y *to a term* y' *which is the representative of the equivalence class w.r.t.* $id_{(\lambda,\vec{a})}$ *to which* y *belongs;* $\tau(x) = x$, *for every* $x \in terms(Q) \setminus \vec{y}$.

Definition 16. *Let* $(\lambda, \vec{a})$ *be an adorned match for* Q *over* $\mathcal{M}_c$. *We denote with* $\rightsquigarrow_{(\lambda,\vec{a})}$: $terms(Q) \times \vec{y}$ *the smallest binary relation containing the pairs* (s, t), *for which there exists an adorned atom* $R^f(s,t) \in (\psi(\vec{x}, \vec{y}))^{\vec{a}}_n$, *such that* $NI(\lambda(t)) \notin \mathcal{M}_c$.

Lemma 8. *Let* $(\lambda, \vec{a})$ *be a fork-free, non-anonymous, and acyclic adorned match for* Q *over* $\mathcal{M}$. *Then* $\rightsquigarrow_{(\lambda,\vec{a})}$ *is acyclic: for every* $t_1, \ldots, t_n \in terms(Q)$, *it is not the case that:* $t_1 \rightsquigarrow_{(\lambda,\vec{a})} t_2 \rightsquigarrow_{(\lambda,\vec{a})} \ldots \rightsquigarrow_{(\lambda,\vec{a})} t_n \rightsquigarrow_{(\lambda,\vec{a})} t_1$.

Proof.

Follows from the fact that $(\lambda, \vec{a})$ is acyclic.

Definition 17. *Let* $(T_i)_{1 \leq i \leq m}$ *be the congruence classes induced by* $\approx$ *over* $terms(\mathcal{M}_c)$, *and let* $(t_i)_{1 \leq i \leq m}$ *be a sequence of terms from* $\mathcal{M}_c$ *s.t. for every* $1 \leq i \leq m$:

1. $t_i \in T_i$,
2. $t_i \in N_I$, *if there exists* $t \in T_i$ *s.t.* $t \in N_i$,

Then, let $\sigma : terms(\mathcal{M}_c) \to terms(\mathcal{M}_c)$ *be the function* $\sigma(t) = t_i$, *for every* $t \in T_i$, *for every* $1 \leq i \leq m$.

Let $(\lambda, \vec{a})$ *be an adorned match for* Q *over* $\mathcal{M}$, *and let* $\textsc{Ini}_{(\lambda,\vec{a})}$ *and* $\textsc{Roots}_{(\lambda,\vec{a})}$ *be the following sets:*

– $\textsc{Ini}_{(\lambda,\vec{a})} = \{t \in terms(Q) \mid \nexists t'.t' \rightsquigarrow_{(\lambda,\vec{a})} t\}$, *and*
– $\textsc{Roots}_{(\lambda,\vec{a})} = \{root(\sigma(\lambda(t))) \mid t \in \textsc{Ini}\}$

Let also ρ_0 : $\textsc{Roots}_{(\lambda,\vec{a})} \to terms(\mathcal{M}_u)$ be some function having the property that: $\rho_0(r) \in \mu(r)$, for every $r \in \textsc{Roots}_{(\lambda,\vec{a})}$, where μ and σ are as in Lemma 5. Furthermore, let $\rho_{(\lambda,\vec{a})} : terms(Q) \to 2^{terms(\mathcal{M}_u)}$ be as follows:

$$\rho_{(\lambda,\vec{a})}(t) = \begin{cases} (\sigma(\lambda(t)))_{r||\rho_0(r)}, & \text{where } r = root(\sigma(\lambda(t))), \text{ if } \tau(t) \in \textsc{Ini}_{(\lambda,\vec{a})}, \\ f^A_{R,B}(\rho_{(\lambda,\vec{a})}(v)), & \text{where } \exists v \text{ s.t. } v \rightsquigarrow_{(\lambda,\vec{a})} \tau(t), \text{ and } \sigma(\lambda(t)) \text{ is} \\ & \text{of type } (A,R,B) \end{cases}$$

Lemma 9. *Let $(\lambda,\vec{a})$ be an adorned match for Q over $\mathcal{M}_c$ that is non-anonymous, fork-free and acyclic and let $\rho_{(\lambda,\vec{a})}$ be as in Definition 17. Then, $\rho_{(\lambda,\vec{a})}$ is a well-defined total function: for every $t \in terms(Q)$, there is a unique value assigned to $\rho_{(\lambda,\vec{a})}(t)$. Furthermore, $\rho_{(\lambda,\vec{a})}(t) \in \mu(\sigma(\lambda(t)))$, for every $t \in terms(Q)$.*

Proof. That each $\rho_{(\lambda,\vec{a})}(t)$ is assigned at least one value, follows from the fact that the guards in Definition 17 cover all possible cases as concerns $\tau(t)$.

It remains to be shown that for each $\rho_{(\lambda,\vec{a})}(t)$, no more than one value is assigned. We first note that:

- $\tau(u) = \tau(v)$ implies $\rho_{(\lambda,\vec{a})}(u) = \rho_{(\lambda,\vec{a})}(v)$ (†): this is the case as all guards in the recursive definition of $\rho'_{(\lambda,\vec{a})}(t)$ concern $\tau(t)$.

Let $rank : terms(Q) \to \mathbb{N}$ be the following function:

$$rank(t) = \begin{cases} 0, & \text{if } \tau(t) \in \textsc{Ini}_{(\lambda,\vec{a})} \\ max\{1 + rank(v) \mid v \rightsquigarrow_{(\lambda,\vec{a})} \tau(t)\}, & \text{otherwise.} \end{cases}$$

Note that $rank$ is well-defined as $\rightsquigarrow_{(\lambda,\vec{a})}$ is acyclic (Lemma 8).

We show the claims of the lemma by induction on $rank(t)$.

For $t \in \textsc{Ini}$, the claims are obvious. We assume that the claims hold for every t such that $rank(t) < k$, where $k > 0$. Let $t \in terms(Q)$ be such that $rank(t) = k > 0$. Then, for every v s.t. $v \rightsquigarrow_{(\lambda,\vec{a})} \tau(t)$, it holds that $f^A_{R,B}(\rho_{\lambda,a}(v)) \in \mu(\sigma(\lambda(t)))$, where $\sigma(\lambda(t))$ is of type (A,R,B). If $\rho_{(\lambda,\vec{a})}(t)$ is not well-defined, there exist v_1, v_2, s.t. $t \rightsquigarrow_{(\lambda,\vec{a})} v_1$ and $t \rightsquigarrow_{(\lambda,\vec{a})} v_2$ and $\rho_{(\lambda,\vec{a})}(v_1) \neq \rho_{(\lambda,\vec{a})}(v_2)$. Then, we distinguish between:

- $\sigma(\lambda(v_1)) \in N_{\mathsf{I}}$; then, from the fact that $(\lambda,\vec{a})$ is fork-free, it follows that $\lambda(v_1) \approx \lambda(v_2)$, and thus: $\sigma(\lambda(v_1)) = \sigma(\lambda(v_2)) \in N_{\mathsf{I}}$. Then, $\mu(\sigma(\lambda(v_1))) = \mu(\sigma(\lambda(v_2))) = \{a\}$. As $rank(v_1), rank(v_2) < rank(t)$, if follows that $\rho_{(\lambda,\vec{a})}(v_1)$ is well-defined and $\rho_{(\lambda,\vec{a})}(v_1) \in \mu(\sigma(\lambda(v_1))) = \{a\}$ and that $\rho_{(\lambda,\vec{a})}(v_2)$ is well-defined and $\rho_{(\lambda,\vec{a})}(v_2) \in \mu(\sigma(\lambda(v_2))) = \{a\}$ – contradiction with $\rho_{(\lambda,\vec{a})}(v_1) \neq \rho_{(\lambda,\vec{a})}(v_2)$
- $\sigma(\lambda(v_2)) \notin N_{\mathsf{I}}$; then, from the fact that $(\lambda,\vec{a})$ is fork-free and Definition 15, it follows that $\tau(v_1) = \tau(v_2)$. As $rank(v_1), rank(v_2) < rank(t)$, if follows that $\rho_{(\lambda,\vec{a})}(v_1)$ and $\rho_{(\lambda,\vec{a})}(v_2)$ are well-defined and from (†) it follows that $\rho_{(\lambda,\vec{a})}(v_1) = \rho_{(\lambda,\vec{a})}(v_2)$ – contradiction, again.

Lemma 10. *Let $(\lambda, \vec{a})$ be an adorned match for Q over $\mathcal{M}_c$ that is non-anonymous, fork-free and acyclic, and let $\rho_{(\lambda,\vec{a})}$ be as in Definition 17. Then, $\rho_{(\lambda,\vec{a})}$ is a non-anonymous match for Q over $\mathcal{M}_u$.*

Proof. From the fact that $(\lambda, \vec{a})$ is an adorned match for Q over $\mathcal{M}_c$, it follows that $\mathcal{M}_c \models (\psi(\lambda(\vec{x}), \lambda(\vec{y})))^{\vec{a}}$, and thus, from Lemma 6: $\mathcal{M}_c \models (\psi(\lambda(\vec{x}), \lambda(\vec{y})))^{\vec{a}}_n$.

We analyse different types of atoms which occur in $(\psi(\lambda(\vec{x}), \lambda(\vec{y})))^{\vec{a}}_n$:

- Assume $A_i(\lambda(t_i)) \in \mathcal{M}_c$. Then $A_i(\sigma(\lambda(t_i))) \in \mathcal{M}_c$, and from Lemma 5 ii) it follows that $A_i(u) \in \mathcal{M}_u$, for every $u \in \mu(\sigma(\lambda(t_i)))$. But $\rho_{(\lambda,\vec{a})}(t_i) \in \mu(\sigma(\lambda(t_i)))$ (from Lemma 9), thus $A_i(\rho_{(\lambda,\vec{a})}(t_i)) \in \mathcal{M}_u$.
- Assume $R^f(\lambda(t_1), \lambda(t_2)) \in \mathcal{M}_c$ and $NI(t_2) \notin \mathcal{M}_c$. Then $R^f(\sigma(\lambda(t_1)), \sigma(\lambda(t_2))) \in \mathcal{M}_c$ and $\sigma(t_2) \notin N_I$ and from Lemma 5 iii) it follows that $R(u, f_{R,B}(u)) \in \mathcal{M}_u$, for every $u \in \mu(\sigma(\lambda(t_1)))$, where $\sigma(\lambda(t_2)) = v^i_{R,B}$. Then, $\rho_{(\lambda,\vec{a})}(t_1) \in \mu(\sigma(\lambda(t_1)))$ (from Lemma 9) and $\rho_{(\lambda,\vec{a})}(t_2) = f_{R,B}(\ \rho_{(\lambda,\vec{a})}(t_1))$. Thus, it holds that $R(\rho_{(\lambda,\vec{a})}(t_1), \rho_{(\lambda,\vec{a})}(t_2)) \in \mathcal{M}_u$.
- Assume $R^f(\lambda(t_1), \lambda(t_2)) \in \mathcal{M}_c$ and $NI(t_2) \in \mathcal{M}_c$. Then $R^f(\sigma(\lambda(t_1)), \sigma(\lambda(t_2))) \in \mathcal{M}_c$ and $\sigma(t_2) \in N_I$ and from Lemma 5 iv) it follows that $R(u, \sigma(\lambda(t_2))) \in \mathcal{M}_u$, for every $u \in \mu(\sigma(\lambda(t_1)))$: then $\rho_{(\lambda,\vec{a})}(t_1) \in \mu(\sigma(\lambda(t_1)))$ (from Lemma 9) and $\rho_{(\lambda,\vec{a})}(t_2) = \sigma(\lambda(t_2))$. Thus, $R(\rho_{(\lambda,\vec{a})}(t_1), \rho_{(\lambda,\vec{a})}(t_2)) \in \mathcal{M}_u$.
- Assume $R(\lambda(t_1), \lambda(t_2)) \in \mathcal{M}_c$, $NI(t_1) \in \mathcal{M}_c$, and $NI(t_2) \in \mathcal{M}_c$: then, it is the case that $R(\sigma(\lambda(t_1)), \sigma(\lambda(t_2))) \in \mathcal{M}_u$. But $\rho_{(\lambda,\vec{a})}(t_1) = \sigma(\lambda(t_1))$ and $\rho_{(\lambda,\vec{a})}(t_2) = \sigma(\lambda(t_2))$, thus $R(\rho_{(\lambda,\vec{a})}(t_1), \rho_{(\lambda,\vec{a})}(t_2)) \in \mathcal{M}_u$.

Lemma 11. *For a given substitution $\lambda : \vec{x} \to terms(\mathcal{M})$, it is the case that $\vec{x} \in cert(Q, \mathcal{O})$ iff there exists a match λ' for Q over $\mathcal{M}_u$ where λ' is a homomorphism that extends λ to $terms(Q)$.*

Definition 18. *Let $(T'_i)_{1 \le i \le m}$ be the congruence classes induced by $\approx$ over $terms(\mathcal{M}_u)$, and let $(t'_i)_{1 \le i \le m}$ be a sequence of terms from $\mathcal{M}_u$ s.t. for every $1 \le i \le m$:*

1. $t'_i \in T'_i$,
2. $t'_i \in N_I$*, if there exists* $t' \in T_i$ *s.t.* $t' \in N_i$.

Then, let $\xi : terms(\mathcal{M}_u) \to terms(\mathcal{M}_u)$ be such that $\xi(t) = t'_i$, if $t \in T'_i$ and let $\sigma : terms(\mathcal{M}_u) \to terms(\mathcal{M}_u)$ be a function which has the following properties:

$$\sigma(t) = \begin{cases} \xi(t), & \text{if } \xi(t) \in N_I \\ f(\sigma(u)), & \text{if } \xi(t) = f(u) \end{cases}$$

Also, let $\theta : terms(\mathcal{M}_u) \to terms(\mathcal{M}_c)$ be the following function:

$$\theta(t) = \begin{cases} t, & \text{if } t \in N_I \\ f^A_{R,B}(\theta(u)), & \text{if } t = f^A_{R,B}(u) \text{ and } R \text{ is unsafe}, \\ v^{A,0}_{R,B} & \text{if } t = f^A_{R,B}(u), R \text{ is safe, and } \theta(u) \notin unfold(A,R,B), \\ v^{A,i+1}_{R,B} & \text{if } t = f^A_{R,B}(u), R \in confl(R), \text{ and } \theta(u) = v^{A,i}_{R,B}, \text{ for } i = 0,1 \\ v^{A,1}_{R,B} & \text{if } t = f^A_{R,B}(u) \text{ and } \theta(u) \in cycle(A,R,B). \end{cases}$$

Lemma 12. *Let σ be as in Definition 18. Then for every $t, t_1, t_2 \in terms(\mathcal{M}_u)$, it holds that:*

1. $\sigma(t) \approx t \in \mathcal{M}_u$
2. $\sigma(f(t)) \approx f(\sigma(t)) \in \mathcal{M}_u$
3. $t_1 \approx t_2 \in \mathcal{M}_u$ *implies* $\sigma(t_1) \approx \sigma(t_2) \in \mathcal{M}_u$
4. $\sigma(f(t)) = h(\sigma(t))$ *or* $\sigma(f(t)) \in N_{\mathsf{I}}$.

Proof. For a term $t \in terms(\mathcal{M}_u)$, let:

$$depth_u(t) = \begin{cases} 0, & \text{if } \xi(t) \in N_{\mathsf{I}} \\ 1 + depth_u(u), & \text{if } \xi(t) = f(u) \end{cases}$$

1. We show by induction on $depth_u(t)$ that $\sigma(t) \approx t \in \mathcal{M}_u$. If $depth_u(t) = 0$, $\sigma(t) = \xi(t)$ and $\xi(t) \approx t \in \mathcal{M}_u$. If $depth_u(t) > 0$, $\sigma(t) = f(\sigma(u))$, where $\xi(t) = f(u)$, and from the IH $\sigma(u) \approx u \in \mathcal{M}_u$. Then $f(\sigma(u)) \approx f(u) = \xi(t) \in \mathcal{M}_u$. As $\xi(t) \approx t \in \mathcal{M}_u$, it follows that $\sigma(t) \approx t \in \mathcal{M}_u$.
2. From point 1. above, $\sigma(f(t)) \approx f(t) \in \mathcal{M}_u$. Furthermore, as $t \approx \sigma(t) \in \mathcal{M}_u$, it follows that $f(t) \approx f(\sigma(t)) \in \mathcal{M}_u$. Thus, $\sigma(f(t)) \approx f(\sigma(t)) \in \mathcal{M}_u$.
3. follows from the fact that $\xi(t_1) = \xi(t_2)$, for $t_1 \approx t_2 \in \mathcal{M}_u$.
4. Assume $\xi(f(t)) = h(u)$. Then, $f(t) \approx h(u) \in \mathcal{M}_u$ and from Lemma 2 it follows that $t \approx u \in \mathcal{M}_u$. Then, $\sigma(f(t)) = h(\sigma(u)) = h(\sigma(t))$ or $\sigma(f(t)) \in N_{\mathsf{I}}$.

Lemma 13. *Let σ be as defined in Definition 18. Then $R(\sigma(t_1), \sigma(t_2)) \in \mathcal{M}_u$ implies: $\sigma(t_1) = f_{R,B}(\sigma(t_2))$ or $\sigma(t_2) = f_{R,B}(\sigma(t_1))$ or $\sigma(t_1) \in N_{\mathsf{I}}$ or $\sigma(t_2) \in N_{\mathsf{I}}$, for some $f_{R,B}$.*

Proof. From the fact that $R(\sigma(t_1), \sigma(t_2)) \in \mathcal{M}_u$, there must be a rule in $\pi(\mathcal{O})^{\approx,\top}$:

1. $A(x) \rightarrow R(x, f^A_{R,B}(x))$ such that $A(t_1) \in \mathcal{M}_u$ and $t_2 = f^A_{R,B}(t_1)$. Then, from Lemma 12 it follows that $\sigma(t_2) = h(\sigma(t_1))$ or $\sigma(t_2) \in N_{\mathsf{I}}$.
2. $S(x, y) \rightarrow R(x, y)$ such that $S(t_1, t_2) \in \mathcal{M}_u$. The claim follows directly from the IH.
3. $\mathsf{Inv}(R)(y, x) \rightarrow R(x, y)$ such that $\mathsf{Inv}(R)(t_2, t_1) \in \mathcal{M}_u$. The claim follows directly from the symmetry of the IH.
4. $R(x, z) \wedge z \approx y \rightarrow R(x, y)$ and a term t_3 such that $R(t_1, t_3) \in \mathcal{M}_u$ and $t_3 \approx t_2 \in \mathcal{M}_u$. Then, $\sigma(t_3) = \sigma(t_2)$ and the claim follows from the IH.
5. $R(x, y) \wedge x \approx z \rightarrow R(x, z))$ and a term t_3 such that $R(t_3, t_2) \in \mathcal{M}_u$ and $t_1 \approx t_3 \in \mathcal{M}_u$. Then, $\sigma(t_3) = \sigma(t_1)$ and the claim follows from the IH.

Lemma 14. *Let σ and θ be as in Definition 18. Then, for every $t, t_1, t_2 \in terms(\mathcal{M}_u)$:*

i) $A(t) \in \mathcal{M}_u$ *implies* $A(\theta(\sigma(t))) \in \mathcal{M}_c$,
ii) $R(t_1, t_2) \in \mathcal{M}_u$ *implies* $R(\theta(\sigma(t_1)), \theta(\sigma(t_2))) \in \mathcal{M}_c$,
iii) $t_1 \approx t_2 \in \mathcal{M}_u$ *implies* $\theta(t_1) \approx \theta(t_2) \in \mathcal{M}_c$.

Proof.

From Lemma 12 it follows that:

i) $A(t) \in \mathcal{M}_u$ implies $A(\sigma(t)) \in \mathcal{M}_u$,
ii) $R(t_1, t_2) \in \mathcal{M}_u$ implies $R(\sigma(t_1), \sigma(t_2)) \in \mathcal{M}_u$.

In the following we show by induction on the derivation level of atoms in $\mathcal{M}_u$ that:

i) $A(t) \in \mathcal{M}_u$ implies $A(\theta(t)) \in \mathcal{M}_c$,
ii) $R(t_1, t_2) \in \mathcal{M}_u$ implies $R(\theta(t_1), \theta(t_2)) \in \mathcal{M}_c$,
iii) $t_1 \approx t_2 \in \mathcal{M}_u$ implies $\theta(t_1) \approx \theta(t_2) \in \mathcal{M}_c$.

Let a be in atom in $\mathcal{M}_u$. We distinguish between:

i) $a = A(t)$. Then there must be a rule in $\pi(\mathcal{O})^{\approx,\top}$:
1. $B(x) \to R(x, f^B_{R,A}(x)) \wedge A(f^B_{R,A}(x))$ and a term u such that $B(u) \in \mathcal{M}_u$ and $t = f^B_{R,A}(u)$. Then, from the IH: $B(\theta(u)) \in \mathcal{M}_c$ and $E_\mathcal{O}$ must contain a rule:
   - $B(x) \to R(x, f^B_{R,A}(x)) \wedge A(f^B_{R,A}(x))$ if R is unsafe: then $A(f^B_{R,A}(\theta(u))$ $= A(\ \theta(f^B_{R,A}(u))) = A(\theta(t)) \in \mathcal{M}_c$;
   - $B(x) \to R(x, v^{B,0}_{R,A}) \wedge A(v^{B,0}_{R,A})$ if $\theta(u) \notin unfold(B, R, A)$: then $v^{B,0}_{R,A} = \theta(f^B_{R,A}(u)) = \theta(t)$ and $A(\theta(t)) \in \mathcal{M}_c$;
   - $B(x) \to R(x, v^{B,1}_{R,A}) \wedge A(v^{B,1}_{R,A})$ if $\theta(u) \in cycle(B, R, A)$: similar to the previous case;
   - $B(v^{B,i}_{R,A}) \to R(v^{B,i}_{R,A}, v^{B,i+1}_{R,A}) \wedge A(v^{B,i+1}_{R,A})$ if $\theta(u) = v^{B,i}_{R,A}$ and $R \in confl(R)$: similar to the previous case;
2. $R(x, y) \wedge B(y) \to A(y)$ and a term u s.t. $R(t, u), B(u) \in \mathcal{M}_u$: straightforward application of the IH.
3. $B_1(x) \wedge \ldots B_n(x) \to A(x)$ s.t. $B_1(t), \ldots B_n(t) \in \mathcal{M}_u$: straightforward application of the IH.
4. $A(x), x \approx y \to A(y)$ and a term u s.t. $A(u), u \approx t \in \mathcal{M}_u$: straightforward application of the IH.

ii) $a = R(t_1, t_2)$. Then there must be a rule in $\pi(\mathcal{O})^{\approx,\top}$:
1. $B(x) \to R(x, f^B_{R,A}(x)) \wedge A(f^B_{R,A}(x))$ and a term u such that $B(u) \in \mathcal{M}_u$ and $t = f^B_{R,A}(u)$: similar to case i)1. above.
2. $S(x, y) \to R(x, y)$: straightforward application of the IH.
3. $\mathsf{Inv}(R)(y, x) \to R(x, y)$: straightforward application of the IH.
4. $R(x, y) \wedge y \approx z \to R(x, z)$ and a term u such that $R(t_1, u), u \approx t_2 \in \mathcal{M}_u$: straightforward application of the IH.
5. $R(z, y) \wedge x \approx z \to R(x, y)$ and a term u such that $R(u, t_2), t_1 \approx u \in \mathcal{M}_u$: straightforward application of the IH.

iii) $a = t_1 \approx t_2$: similar to case ii) above.

Lemma 15. *Let σ and θ be as defined in Definition 18. Then, for every $t, t_1, t_2 \in terms(\mathcal{M}_u)$:*

i) $R(t_1, t_2) \in \mathcal{M}_u$*,* $\sigma(t_1) < \sigma(t_2)$*, and* $\sigma(t_1) \notin N_I$ *implies* $R^f(\theta(\sigma(t_1)), \theta(\sigma(t_2))) \in \mathcal{M}_c$.

ii) $R(t_1,t_2) \in \mathcal{M}_u$, $\sigma(t_1) < \sigma(t_2)$, *and* $\sigma(t_1) \in N_I$ *implies* $R^f(\theta(\sigma(t_1)), \theta(\sigma(t_2))) \in \mathcal{M}_c$ *or* $R^b(\theta(\sigma(t_1)), \theta(\sigma(t_2))) \in \mathcal{M}_c$.

iii) $R(t_1,t_2) \in \mathcal{M}_u$, $\sigma(t_1) \not< \sigma(t_2)$, $\sigma(t_1) \in N_I$, *and* $\sigma(t_2) \notin N_I$ *implies* $R^b(\theta(\sigma(t_1)), \theta(\sigma(t_2))) \in \mathcal{M}_c$.

iv) $R(t_1,t_2) \in \mathcal{M}_u$, $\sigma(t_2) < \sigma(t_1)$, *and* $\sigma(t_2) \notin N_I$ *implies* $R^b(\theta(\sigma(t_1)), \theta(\sigma(t_2))) \in \mathcal{M}_c$.

v) $R(t_1,t_2) \in \mathcal{M}_u$, $\sigma(t_2) < \sigma(t_1)$, *and* $\sigma(t_2) \in N_I$ *implies* $R^f(\theta(\sigma(t_1)), \theta(\sigma(t_2))) \in \mathcal{M}_c$ *or* $R^b(\theta(\sigma(t_1)), \theta(\sigma(t_2))) \in \mathcal{M}_c$.

vi) $R(t_1,t_2) \in \mathcal{M}_u$, $\sigma(t_2) \not< \sigma(t_1)$, $\sigma(t_2) \in N_I$, *and* $\sigma(t_1) \notin N_I$ *implies* $R^f(\theta(\sigma(t_1)), \theta(\sigma(t_2))) \in \mathcal{M}_c$.

Proof. We show that the claims of the lemma hold by induction on the derivation level of atoms in $\mathcal{M}_u$.

Let a be in atom in $\mathcal{M}_u$. We distinguish between:

i) $a = R(t_1,t_2)$, with $\sigma(t_1) < \sigma(t_2)$, and $\sigma(t_1) \notin N_\mathsf{I}$. Then there must be a rule in $\pi(\mathcal{O})^{\approx,\top}$:

1. $A(x) \to R(x, f^A_{R,B}(x)) \wedge B(f^A_{R,B}(x))$, with $A(t_1) \in \mathcal{M}_u$ and $t_2 = f^A_{R,B}(t_1)$. From Lemma 14 $A(\theta(\sigma(t_1))) \in \mathcal{M}_c$ and one of the following holds:
   - R is unsafe and E_O contains a rule $A(x) \to R^f(x, f^A_{R,B}(x)) \wedge B(\, f^A_{R,B}(x))$. Then $R^f(\theta(\sigma(t_1)), f^A_{R,B}(\theta(\sigma(t_1)))) \in \mathcal{M}_c$. But, $f^A_{R,B}(\theta(\sigma(t_1))) = \theta(f^A_{R,B}(\sigma(t_1)))$, from Lemma 12, $f^A_{R,B}(\sigma(t_1)) \approx \sigma(f^A_{R,B}(t_1)) \in \mathcal{M}_c$, and $f^A_{R,B}(t_1) = t_2$. Thus, $f^A_{R,B}(\theta(\sigma(t_1))) \approx \theta(\sigma(t_2))$, and $R^f(\theta(\sigma(t_1)), \theta(\sigma(t_2))) \in \mathcal{M}_c$.
   - R is safe and E_O contains a rule $A(x) \wedge notIn(x, unfold(A,R,B)) \to R^f(x, v^{A,0}_{R,B}) \wedge B(v^{A,0}_{R,B})$, and $\theta(\sigma(t_1)) \notin unfold(A,R,B)$. Then, $\theta(\sigma(t_2)) = \theta(\sigma(f^A_{R,B}(t_1))) \approx \theta(f^A_{R,B}(\sigma(t_1))) = v^{A,0}_{R,B} \in \mathcal{M}_c$ and. Thus, $R^f(\theta(\sigma(t_1)), \theta(\sigma(t_2))) \in \mathcal{M}_c$.
   - R is safe and E_O contains a rule $A(x) \to R^f(x, v^{A,1}_{R,B}) \wedge B(v^{A,1}_{R,B})$, and $\theta(\sigma(t_1)) \in cycle(A,R,B)$. Similar to above.
   - $R \in confl(R)$ and E_O contains a rule $A(v^{A,i}_{R,B}) \to R^f(v^{A,i}_{R,B}, v^{A,i+1}_{R,B}) \wedge B(v^{A,i+1}_{R,B})$, and $\theta(\sigma(t_1)) = v^{A,i}_{R,B}$. Similar to above.
2. $S(x,y) \to R(x,y)$ with $S(t_1,t_2) \in \mathcal{M}_u$. From the IH, $S^f(\theta(\sigma(t_1)), \theta(\sigma(t_2)) \in \mathcal{M}_c$, and E_O contains a rule: $S^f(x,y) \to R^f(x,y)$, thus $R^f(\theta(\sigma(t_1)), \theta(\sigma(t_2)) \in \mathcal{M}_c$.
3. $\mathsf{Inv}(R)(y,x) \to R(x,y)$ with $\mathsf{Inv}(R)(t_2,t_1) \in \mathcal{M}_u$. From the IH: $\mathsf{Inv}(R)^b(\theta(\sigma(t_2)), \theta(\sigma(t_1)) \in \mathcal{M}_c$, and thus $R^f(\theta(\sigma(t_1)), \theta(\sigma(t_2)) \in \mathcal{M}_c$.
4. $R(x,y), z \approx y \to R(x,z)$, and term t_3 s.t. $R(t_1,t_3), t_3 \approx t_2 \in \mathcal{M}_u$. Then, from Lemma 12 $\sigma(t_3) = \sigma(t_2)$ and thus, one can apply the IH to $R(t_1,t_3)$: $R^f(\theta(\sigma(t_1)), \theta(\sigma(t_3))) \in \mathcal{M}_c$.
5. $R(z,y), z \approx x \to R(x,y)$, and term t_3 s.t. $R(t_3,t_2), t_3 \approx t_1 \in \mathcal{M}_u$. Similar to above.

ii) $a = R(t_1,t_2)$, with $\sigma(t_1) < \sigma(t_2)$, and $\sigma(t_1) \in N_\mathsf{I}$: similar to case i).

iii) $a = R(t_1,t_2)$, with $\sigma(t_1) \not< \sigma(t_2)$, $\sigma(t_1) \in N_\mathsf{I}$, and $\sigma(t_2) \notin N_\mathsf{I}$. Then there must be a rule in $\pi(\mathcal{O})^{\approx,\top}$:

1. $A(x) \to R(x, f^A_{R,B}(x)) \wedge B(f^A_{R,B}(x))$, with $A(t_1) \in \mathcal{M}_u$ and $t_2 = f^A_{R,B}(t_1)$. But then, from Lemma 12 it follows that $\sigma(t_2) = h(\sigma(t_1))$ or $\sigma(t_2) \in N_\mathsf{I}$ –contradiction with the original assumptions
2. $S(x, y) \to R(x, y)$ – similar to case i) 2.
3. $\mathsf{Inv}(R)(y, x) \to R(x, y)$ – similar to case i) 3.
4. $R(x, y) \wedge y \approx z \to R(x, z)$ – similar to case i) 4.
5. $R(z, y) \wedge x \approx z \to R(x, y)$ – similar to case i) 5.

iv) $a = R(t_1, t_2) \in \mathcal{M}_u$, with $\sigma(t_2) < \sigma(t_1)$, and $\sigma(t_2) \notin N_\mathsf{I}$. Similar to case iii).
v) $a = R(t_1, t_2) \in \mathcal{M}_u$, with $\sigma(t_2) < \sigma(t_1)$, and $\sigma(t_2) \in N_\mathsf{I}$. Similar to case ii).
vi) $R(t_1, t_2) \in \mathcal{M}_u$, with $\sigma(t_2) \not< \sigma(t_1)$, $\sigma(t_2) \in N_\mathsf{I}$, and $\sigma(t_1) \notin N_\mathsf{I}$. Similar to case i).

Definition 19. *For a term $t \in terms(\mathcal{M}_c)$, let:*

$$depth_c(t) = \begin{cases} 1 + depth_c(u), & \text{if } t = f(u) \text{ and } t \not\approx a, \text{ for any } a \in N_I \\ 0, & \text{otherwise} \end{cases}$$

Lemma 16. *For every $t_1, t_2 \in terms(\mathcal{M}_c)$: $t_1 \approx t_2$ implies $depth_c(t_1) = depth_c(t_2)$.*

Proof. We fix a term t_1 and show by induction on $depth_c(t_1)$ that for every $t_2 \in terms(\mathcal{M}_c)$ s.t. $t_1 \approx t_2 \in \mathcal{M}_c$, $depth_c(t_1) = depth_c(t_2)$. □

Lemma 17. *For every $t \in terms(\mathcal{M}_c)$, concepts A, B, and role R, such that $v^{A,0}_{R,B} \not\approx a$, for every $a \in N_I$, it holds that:*

1. *$t \in cycle(A, R, B)$ and $R^f(t, v^{A,i}_{R,B}) \in \mathcal{M}_c$ implies $i = 1$;*
2. *$t \notin cycle(A, R, B)$ and $R^f(t, v^{A,i}_{R,B}) \in \mathcal{M}_c$ implies $i = 0$.*

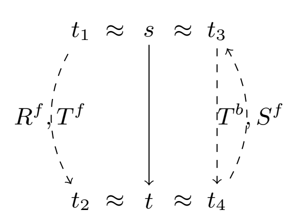

Fig. 6: Ambiguous roles in $\mathcal{M}_c$: both $T^f(s, t)$ and $T^b(s, t)$ hold

Lemma 18. *For any role T and terms s and t, it is not the case that both $T^f(s, t) \in \mathcal{M}_c$ and $T^b(s, t) \in \mathcal{M}_c$.*

Proof. Assume the opposite. Then, there must be some roles R and S and terms t_1, t_2, t_3, and t_4 such that: $R \sqsubseteq^*_{\mathcal{R}} T$, $S \sqsubseteq^*_{\mathcal{R}} \mathsf{Inv}(T)$, $t_1 \approx s \in \mathcal{M}_c$, $t_2 \approx t \in \mathcal{M}_c$, $t_3 \approx s \in \mathcal{M}_c$, $t_4 \approx t \in \mathcal{M}_c$, $R^f(t_1, t_2) \in \mathcal{M}_c$, $S^f(t_4, t_3) \in \mathcal{M}_c$ (see Figure 6), t_2 is of type (A, R, B) and t_3 is of type (D, S, C), for some concepts A, B, C and D.

We first deal with the case where one of t_1, t_2, t_3, and t_4 is equal to a named individual. W.l.o.g., let us assume that $t_1 \approx a \in \mathcal{M}_c$, where $a \in N_\mathsf{I}$. Then, $t_3 \approx a \in \mathcal{M}_c$, as well. From the fact that $R(a, t_2) \in \mathcal{M}_c$ and Lemma 1 it follows that $R(a, u^A_{R,B}) \in M_\mathsf{RSA}$ (1). Further on, $S(t_4, t_3) \in \mathcal{M}_c$ implies $S(t_2, a) \in \mathcal{M}_c$, and thus $S(u^A_{R,B}, a) \in M_\mathsf{RSA}$ (2). From (1), (2), and the fact that $R \sqsubseteq^*_{\mathcal{R}} T$, and $S \sqsubseteq^*_{\mathcal{R}} \mathsf{Inv}(T)$, it follows that $\mathcal{O}$ is not equality-safe – contradiction.

In the following, we assume that none of t_1, t_2, t_3, and t_4 are equal to a named individual. Then, one of the following holds:

- if t_1 is of form $v^{D,i}_{S,C}$, then $t_3 = t_1$ (from Lemma 3). We distinguish between:
  - t_2 is of form $v^{A,i}_{R,B}$: then $t_4 = t_2$ (from Lemma 3) and all of the following hold:
    - if $(A, R, B) \prec (D, S, C)$: $\begin{cases} t_1 = v^{D,0}_{S,C} \\ t_2 = v^{A,1}_{R,B} \end{cases}$ or $\begin{cases} t_1 = v^{D,1}_{S,C} \\ t_2 = v^{A,0}_{R,B} \end{cases}$. At the same time: $\begin{cases} t_3 = v^{D,0}_{S,C} \\ t_4 = v^{A,0}_{R,B} \end{cases}$ or $\begin{cases} t_1 = v^{D,1}_{S,C} \\ t_2 = v^{A,1}_{R,B} \end{cases}$. This is in contradiction to the fact that $t_1 = t_3$ and $t_2 = t_4$.
    - if $(D, S, C) \prec (A, R, B)$: similar to the previous case.
  - $t_2 = f^A_{R,B}(t_1)$ and R is unsafe. Then, $S^f(f^A_{R,B}(t_1), t_1) = S^f(f^A_{R,B}(v^{D,i}_{S,C}), v^{D,i}_{S,C}) \in \mathcal{M}_c$. If $i = 0$, $f^A_{R,B}(v^{D,0}_{S,C}) \in \mathit{cycle}(D, S, C)$, and from Lemma 17, $S^f(f^A_{R,B}(v^{D,0}_{S,C}), v^{D,0}_{S,C}) \notin \mathcal{M}_c$ – contradiction. If $i = 1$, $f^A_{R,B}(v^{D,1}_{S,C}) \notin \mathit{cycle}(D, S, C)$. Thus, by applying Lemma 17, $S^f(f^A_{R,B}(v^{D,1}_{S,C}), v^{D,1}_{S,C}) \notin \mathcal{M}_c$ – contradiction.
- if both t_1 and t_2 are functional, t_3 and t_4 are functional as well, and furthermore $t_2 = f^A_{R,B}(t_1)$ and $t_3 = f^D_{S,C}(t_4)$. From Lemma 16 it follows that: $\mathit{depth}_c(t_1) = \mathit{depth}_c(t_3)$, and $\mathit{depth}_c(t_2) = \mathit{depth}_c(t_4)$. But $\mathit{depth}_c(t_2) = \mathit{depth}_c(t_1) + 1$, and $\mathit{depth}_c(t_3) = \mathit{depth}_c(t_4) + 1$ – contradiction.

Lemma 19. *Let ρ be a non-anonymous match for Q over $\mathcal{M}_u$ and let $\lambda(\cdot) = \theta(\sigma(\rho(\cdot)))$. Furthermore, let $\vec{a}$ be the following adornment for $\psi(\vec{x}, \vec{y})$:*

$$a_j = \begin{cases} \text{␣}, & \text{if } R_j(\lambda(u_{1j}), \lambda(u_{2j})) \in \mathcal{M}_c, \text{ and} \\ & R^f_j(\lambda(u_{1j}), \lambda(u_{2j})), R^b_j(\lambda(u_{1j}), \lambda(u_{2j})) \notin \mathcal{M}_c \\ f, & \text{if } R^f_j(\lambda(u_{1j}), \lambda(u_{2j})) \in \mathcal{M}_c \\ b, & \text{if } R^f_b(\lambda(u_{1j}), \lambda(u_{2j})) \in \mathcal{M}_c. \end{cases}$$

Then $(\lambda, \vec{a})$ is an adorned match for Q over $\mathcal{M}_c$. Furthermore, $(\lambda, \vec{a})$ is non-anonymous, fork-free and acyclic.

Proof. That $(\lambda, \vec{a})$ is an adorned match for Q over $\mathcal{M}_c$, follows from Lemma 15. It is also easy to see that $(\lambda, \vec{a})$ is non-anonymous provided that ρ is non-anonymous.

To see that $(\lambda, \vec{a})$ is acyclic, assume the contrary. Then, there exists a sequence $R^f_{o_1}(y_{l_1}, y_{l_2}), R^f_{o_2}(y_{l_3}, y_{l_4}), \ldots, R^f_{o_p}(y_{l_{2p-1}}, y_{l_{2p}}) \in (\psi(\vec{x}, \vec{y}))^{\vec{a}}_n$, such that:

1. $\mathsf{id}(\lambda(\vec{x}), \lambda(\vec{y}), l_{2i}, l_{2i+1}) \in \mathcal{M}$, for every $1 \leq i \leq p$ ($l_{2p+1} = l_1$), and
2. $NI(\lambda(y_{l_j})) \notin \mathcal{M}$, for every $1 \leq j \leq 2p$.

Let $s_i = \sigma(\rho(y_{l_{2i}}))$, for $1 \leq i \leq p$. Then: $R_{o_1}(s_p, s_1), R_{o_2}(s_1, s_2), \ldots, R_{o_p}(s_{p-1}, s_p) \in \mathcal{M}_u$, where $s_i \notin N_{\mathsf{I}}$, for every $1 \leq i \leq p$. Then, from Lemma 15 and Lemma 18, and $R^f_{o_i}(\theta(s_i), \theta(s_{i+1})) \in \mathcal{M}_c$, for every $1 \leq i \leq p$, it follows that $s_i < s_{i+1}$, for every $1 \leq i \leq p$ - thus $s_i < s_i$ – contradiction.

To see that $(\lambda, \vec{a})$ is fork-free, we assume again the contrary. Then, there must be a pair of atoms $R^f(u, y_i), S^f(v, y_j) \in (\psi(\vec{x}, \vec{y}))^{\vec{a}}_n$, such that $u, v \in \vec{x} \cup \vec{y}$, $y_i, y_j \in \vec{y}$, and $\mathsf{id}(\lambda(\vec{x}), \lambda(\vec{y}), i, j) \in \mathcal{M}$, and $\lambda(u) \not\approx \lambda(v)$.

From the fact that $\mathsf{id}(\lambda(\vec{x}), \lambda(\vec{y}), i, j) \in \mathcal{M}$, it follows that either:

- $i = j$: then, as $NI(\lambda(y_i)), NI(\lambda(y_j)) \notin \mathcal{M}$, it follows that $NI(\sigma(\rho(y_i))), NI(\sigma(\rho(y_j))) \notin \mathcal{M}_u$, $\sigma(\rho(y_i)) = f_{R,B}(\sigma(\rho(u))$, and $\sigma(\rho(y_j)) = f_{S,C}(\sigma(\rho(v))$. But, as $i = j$, $\sigma(\rho(y_i)) = \sigma(\rho(y_j))$, and thus $f_{R,B}$ and $f_{S,C}$ must be in fact the same function symbol, and $\sigma(\rho(u)) = \sigma(\rho(v))$. Then: $\lambda(u) = \lambda(v)$ – contradiction.
- or there exist two sequences of atoms:
  - $R^f_{l_1}(y_i, y_{l_1}), \ldots, R^f_{l_m}(y_{l_{m-1}}, y_{l_m})$, and
  - $R^f_{k_1}(y_j, y_{k_1}), \ldots, R^f_{k_m}(y_{k_{m-1}}, y_{k_m})$,

  such that: $l_m = k_m$, and $\mathsf{id}(\lambda(\vec{x}), \lambda(\vec{y}), l_i, k_i) \in \mathcal{M}$, for every $1 \leq i \leq m$.

Then, it can be shown by induction on the length m of the sequences introduced above that $\sigma(\rho(y_{l_i})) = \sigma(\rho(y_{k_i}))$, for every $1 \leq i \leq m$, and then, further on, that $\sigma(\rho(u)) = \sigma(\rho(v))$, and consequently $\lambda(u) = \lambda(v)$ – contradiction.

Theorem 1 and **Theorem 2** recapitulate results related to RSA, thus their proofs can be found in the related publication [4]. The proof sketch for **Theorem 5** is already provided in the paper. As such, we will provide next the proofs for **Theorem 3** and **Theorem 4**.

Theorem 3. *The following holds: (i) $M[E_{\mathcal{O}}]$ is polynomial in $|\mathcal{O}|$ (ii) $\mathcal{O}$ is satisfiable iff $E_{\mathcal{O}} \not\models \exists y.\bot(y)$ (iii) if $\mathcal{O}$ is satisfiable, $\mathcal{O} \models A(c)$ iff $A(c) \in M[E_{\mathcal{O}}]$ and (iv) there are no terms s, t and role R s.t. $E_{\mathcal{O}} \models R^f(s,t) \wedge R^b(s,t)$.*

Proof.

(i) $M[E_{\mathcal{O}}]$ is polynomial in $|\mathcal{O}|$: the size of $E_{\mathcal{O}}$ is linear in $|\mathcal{O}|$ and the number of variables in each rule is bounded by a constant. Thus, the LHM of the program is bounded in size by $|\mathcal{O}|^3$.

(ii) $\mathcal{O}$ is satisfiable iff $E_{\mathcal{O}} \not\models \exists y.\bot(y)$: follows from Lemma 5 and Lemma 15;

(iii) if $\mathcal{O}$ is satisfiable, $\mathcal{O} \models A(c)$ iff $A(c) \in M[E_{\mathcal{O}}]$: follows from Lemma 5 and Lemma 15;

(iv) there are no terms s, t and role R s.t. $E_{\mathcal{O}} \models R^f(s,t) \wedge R^b(s,t)$: see Lemma 18.

Theorem 4. *(i) $\mathcal{P}_{\mathcal{O},Q}$ is stratified; (ii) $M[\mathcal{P}_{\mathcal{O},Q}]$ is polynomial in $|\mathcal{O}|$ and exponential in $|Q|$; and (iii) if $\mathcal{O}$ is satisfiable, $\vec{x} \in cert(Q, \mathcal{O})$ iff $\mathcal{P}_{\mathcal{O},Q} \models \mathsf{Ans}(\vec{x})$.*

Proof.

(i) $\mathcal{P}_{\mathcal{O},Q}$ is stratified: a three-layered stratification of $\mathcal{P}_{\mathcal{O},Q}$ can be constructed as follows:
 - first stratum contains all predicates from $E_{\mathcal{O}}$ as well as predicates NI and QM;
 - second stratum contains predicates $\mathsf{id}, \mathit{fk}, AQ^*, TQ^*$, and sp;
 - third stratum contains predicate Ans.

(ii) $M[\mathcal{P}_{\mathcal{O},Q}]$ is polynomial in $|\mathcal{O}|$ and exponential in $|Q|$: the number of rules in $\mathcal{P}_{\mathcal{O},Q}$ is linear in $|\mathcal{O}|$ and quadratic in $|Q|$. At the same time, the number of variables in these rules is bounded by a constant in $|\mathcal{O}|$ and linearly in $|Q|$ (due to rule **(1)** in $\mathcal{P}_{\mathcal{O},Q}$). Thus, the materialization of $\mathcal{P}_{\mathcal{O},Q}$ is bounded polynomially in $|\mathcal{O}|$ and exponentially in $|Q|$.

(iii) if $\mathcal{O}$ is satisfiable, $\vec{c} \in cert(Q, \mathcal{O})$ iff $\mathcal{P}_{\mathcal{O},Q} \models \mathsf{Ans}(\vec{c})$:
Assume $\mathcal{P}_{\mathcal{O},Q} \models \mathsf{Ans}(\lambda(\vec{x}))$, where $\lambda : \vec{x} \to terms(\mathcal{M})$. Then, according to Lemma 7, there exists an adorned match $(\lambda', \vec{a})$ for Q over $\mathcal{M}$ which is non-anonymous, fork-free, and acyclic, where λ' is a homomorphism that extends λ to $terms(Q)$. Furthermore, according to Lemma 10, $\rho_{(\lambda',\vec{a})}$ is a non-anonymous match for Q over $\mathcal{M}_u$. Note that $\rho_{(\lambda',\vec{a})}$ is such that for every $t \in terms(Q)$, $\rho_{(\lambda',\vec{a})}(t) \in \mu(\sigma(\lambda(t)))$. Thus, $\rho_{(\lambda',\vec{a})}$ does not necessary extend λ. But ρ' obtained from ρ by setting $\rho'(t) = \begin{cases} \lambda'(t) & \text{if } t \in terms(Q) \setminus \vec{y} \\ \rho(t), & \text{otherwise} \end{cases}$ is a homomorphism that extends λ'. At the same time, it is a match for Q over $\mathcal{M}_u$ (note that according to Lemma 5 vii) $t_1 \approx t_2 \in \mathcal{M}$, with $t_1, t_2 \in N_{\mathsf{I}}$ implies $t_1 \approx t_2 \in \mathcal{M}_u$). Then, according to Lemma 11: $\vec{x} \in cert(Q, \mathcal{O})$.
Assume $\vec{x} \in cert(Q, \mathcal{O})$. Then, according to Lemma 11, there exists a match ρ for Q over $\mathcal{M}_u$. According to Lemma 19 one can construct from ρ a match $(\lambda, \vec{a})$ over $\mathcal{M}$ which is non-anonymous, fork-free and acyclic. Again, λ does not necessary preserve the mapping of ρ over $terms(Q) \setminus \vec{y}$. But, λ can be transformed into another mapping λ' such that $\lambda'(t) = \begin{cases} \rho(t), & \text{for every } t \in terms(Q) \setminus \vec{y}, \\ t, & otherwise \end{cases}$. It can be checked that $(\lambda', \vec{a})$ is still non-anonymous, fork-free and acyclic. Then, by applying Lemma 7 we obtain that $\mathcal{P}_{\mathcal{O},Q} \models \mathsf{Ans}(\lambda(\vec{x}))$.