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SAT Encoding of Unification in \mathcal{ELH}_{R^+} w.r.t. Cycle-Restricted Ontologies

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Abstract

Unification in Description Logics has been proposed as an inference service that can, for example, be used to detect redundancies in ontologies. For the Description Logic \mathcal{EL} , which is used to define several large biomedical ontologies, unification is NP-complete. An NP unification algorithm for \mathcal{EL} based on a translation into propositional satisfiability (SAT) has recently been presented. In this report, we extend this SAT encoding in two directions: on the one hand, we add general concept inclusion axioms, and on the other hand, we add role hierarchies (\mathcal{H}) and transitive roles (R^+). For the translation to be complete, however, the ontology needs to satisfy a certain cycle restriction. The SAT translation depends on a new rewriting-based characterization of subsumption w.r.t. \mathcal{ELH}_{R^+} -ontologies.

1 Introduction

The Description Logic (DL) \mathcal{EL} , which offers the constructors conjunction (\sqcap), existential restriction ($\exists r.C$), and the top concept (\top), has recently drawn considerable attention since, on the one hand, important inference problems such as the subsumption problem are polynomial in \mathcal{EL} , even in the presence of general concept inclusion axioms (GCIs) [12, 3]. On the other hand, though quite inexpressive, \mathcal{EL} can be used to define biomedical ontologies, such as the large medical ontology SNOMED CT.¹

Unification in DLs has been proposed in [8] as a novel inference service that can, for instance, be used to detect redundancies in ontologies. For example, assume that one developer of a medical ontology defines the concept of a *patient with severe injury of the frontal lobe* as

$$\exists \text{finding} . (\text{Frontal_lobe_injury} \sqcap \exists \text{severity} . \text{Severe}), \quad (1)$$

¹see <http://www.ihtsdo.org/snomed-ct/>

whereas another one represents it as

$$\exists \text{finding} . (\text{Severe_injury} \sqcap \exists \text{finding_site} . \exists \text{part_of} . \text{Frontal_lobe}). \quad (2)$$

These two concept descriptions are not equivalent, but they are nevertheless meant to represent the same concept. They can obviously be made equivalent by treating the concept names `Frontal_lobe_injury` and `Severe_injury` as variables, and substituting the first one by `Injury` \sqcap `finding_site` \exists `part_of` `Frontal_lobe` and the second one by `Injury` \sqcap `severity` `Severe`. In this case, we say that the descriptions are unifiable, and call the substitution that makes them equivalent a *unifier*.

To motivate our interest in unification w.r.t. GCIs, role hierarchies, and transitive roles, assume that the developers use the descriptions (3) and (4) instead of (1) and (2):

$$\begin{aligned} & \exists \text{finding} . \exists \text{finding_site} . \exists \text{part_of} . \text{Brain} \sqcap \\ & \exists \text{finding} . (\text{Frontal_lobe_injury} \sqcap \exists \text{severity} . \text{Severe}) \end{aligned} \quad (3)$$

$$\begin{aligned} & \exists \text{status} . \text{Emergency} \sqcap \\ & \exists \text{finding} . (\text{Severe_injury} \sqcap \exists \text{finding_site} . \exists \text{part_of} . \text{Frontal_lobe}) \end{aligned} \quad (4)$$

The descriptions (3) and (4) are not unifiable without additional background knowledge, but they are unifiable, with the same unifier as above, if the GCIs

$$\begin{aligned} \exists \text{finding} . \exists \text{severity} . \text{Severe} & \sqsubseteq \exists \text{status} . \text{Emergency}, \\ \text{Frontal_lobe} & \sqsubseteq \exists \text{proper_part_of} . \text{Brain} \end{aligned}$$

are present in a background ontology and this ontology additionally states that `part_of` is transitive and `proper_part_of` is a subrole of `part_of`.

Most of the previous results on unification in DLs did not consider such additional background knowledge. In [8] it was shown that, for the DL \mathcal{FL}_0 , which differs from \mathcal{EL} by offering value restrictions ($\forall r.C$) in place of existential restrictions, deciding unifiability is an ExpTime-complete problem. In [5], we were able to show that unification in \mathcal{EL} is of considerably lower complexity: the decision problem is NP-complete. The original unification algorithm for \mathcal{EL} introduced in [5] was a brutal “guess and then test” NP-algorithm, but we have since then also developed more practical algorithms. On the one hand, in [7] we describe a goal-oriented unification algorithm for \mathcal{EL} , in which nondeterministic decisions are only made if they are triggered by “unsolved parts” of the unification problem. On the other hand, in [6], we present an algorithm that is based on a reduction to satisfiability in propositional logic (SAT). In [7] it was also shown that the approaches for unification of \mathcal{EL} -concept descriptions (without any background ontology) can easily be extended to the case of an acyclic TBox as background ontology without really changing the algorithms or increasing their complexity. Basically, by viewing defined concepts as variables, an acyclic TBox can be turned

into a unification problem that has as its unique unifier the substitution that replaces the defined concepts by unfolded versions of their definitions.

For GCIs, this simple trick is not possible, and thus handling them requires the development of new algorithms. In [1, 2] we describe two such new algorithms: one that extends the brute-force “guess and then test” NP-algorithm from [5] and a more practical one that extends the goal-oriented algorithm from [7]. Both algorithms are based on a new characterization of subsumption w.r.t. GCIs in \mathcal{EL} , which we prove using a Gentzen-style proof calculus for subsumption. Unfortunately, these algorithms are complete only for cycle-restricted TBoxes, i.e., finite sets of GCIs that satisfy a certain restriction on cycles, which, however, does not prevent all cycles. For example, the cyclic GCI $\exists\text{child.Human} \sqsubseteq \text{Human}$ satisfies this restriction, whereas the cyclic GCI $\text{Human} \sqsubseteq \exists\text{parent.Human}$ does not.

In this report, we still cannot get rid of cycle-restrictedness of the ontology, but extend the results of [2] in two other directions: (i) we add transitive roles (indicated by the subscript R^+ in the name of the DL) and role hierarchies (indicated by adding the letter \mathcal{H} to the name of the DL) to the language, which are important for medical ontologies [22, 20]; (ii) we provide an algorithm that is based on a translation into SAT, and thus allows us to employ highly optimized state-of-the-art SAT solvers [11] for implementing the unification algorithm. In order to obtain the SAT translation, using the characterization of subsumption from [2] is not sufficient, however. We had to develop a new rewriting-based characterization of subsumption.

In the next section, we introduce the DLs considered in this report and the important inference problem subsumption. In Section 3 we then derive rewriting-based characterizations of subsumption. In Section 4 we define unification for the considered DLs and recall some of the existing results for unification in \mathcal{EL} . In particular, we introduce in this section the notion of cycle-restrictedness, which is required for the results on unification w.r.t. GCIs to hold. Section 5 contains the main result, which is a reduction of unification in \mathcal{ELH}_{R^+} w.r.t. cycle-restricted ontologies to propositional satisfiability. The proof of correctness of this reduction strongly depends on the characterization of subsumption shown before.

2 Preliminaries

The expressiveness of a DL is determined both by the formalism for describing concepts (the concept description language) and the terminological formalism, which can be used to state additional constraints on the interpretation of concepts and roles in a so-called ontology.

Name	Syntax	Semantics
concept name	A	$A^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}}$
role name	r	$r^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}} \times \Delta^{\mathcal{I}}$
top	\top	$\top^{\mathcal{I}} = \Delta^{\mathcal{I}}$
conjunction	$C \sqcap D$	$(C \sqcap D)^{\mathcal{I}} = C^{\mathcal{I}} \cap D^{\mathcal{I}}$
existential restr.	$\exists r.C$	$(\exists r.C)^{\mathcal{I}} = \{x \mid \exists y : (x, y) \in r^{\mathcal{I}} \wedge y \in C^{\mathcal{I}}\}$
concept def.	$A \equiv C$	$A^{\mathcal{I}} = C^{\mathcal{I}}$
GCI	$C \sqsubseteq D$	$C^{\mathcal{I}} \subseteq D^{\mathcal{I}}$
role inclusion	$r_1 \circ \dots \circ r_n \sqsubseteq s$	$r_1^{\mathcal{I}} \circ \dots \circ r_n^{\mathcal{I}} \subseteq s^{\mathcal{I}}$

Table 1: Syntax and semantics of \mathcal{EL} .

2.1 Syntax and Semantics of \mathcal{EL}

The concept description language considered in this report is called \mathcal{EL} . Starting with a finite set N_C of *concept names* and a finite set N_R of *role names*, \mathcal{EL} -*concept descriptions* are built from concept names by the constructors *conjunction* ($C \sqcap D$), *existential restriction* ($\exists r.C$ for every $r \in N_R$), and *top* (\top). We say that a concept description C is *built over a signature* $\Sigma \subseteq N_C \cup N_R$ if only concept and role names from Σ occur in it. Since we only consider \mathcal{EL} -concept descriptions, we will sometimes dispense with the prefix \mathcal{EL} .

An *interpretation* $\mathcal{I} = (\Delta^{\mathcal{I}}, \cdot^{\mathcal{I}})$ consists of a non-empty domain $\Delta^{\mathcal{I}}$ and an interpretation function that maps concept names to subsets of $\Delta^{\mathcal{I}}$ and role names to binary relations over $\Delta^{\mathcal{I}}$. This function is extended to concept descriptions as shown in the semantics column of Table 1.

2.2 Ontologies

A *concept definition* is of the form $A \equiv C$ for a concept name A and a concept description C , and a *general concept inclusion (GCI)* is of the form $C \sqsubseteq D$ for concept descriptions C, D . A *role inclusion* is of the form $r_1 \circ \dots \circ r_n \sqsubseteq s$ for role names r_1, \dots, r_n, s . All three are called *axioms*. Role inclusions of the form $r \circ r \sqsubseteq r$ are called *transitivity axioms* and of the form $r \sqsubseteq s$ *role hierarchy axioms*. An interpretation \mathcal{I} *satisfies* such an axiom if the corresponding condition in the semantics column of Table 1 holds, where \circ in this column stands for composition of binary relations.

An \mathcal{EL}^+ -*ontology* is a finite set of axioms. We will often write an ontology in the form $(\mathcal{T}, \mathcal{R})$, where the *TBox* \mathcal{T} consists of finitely many concept definitions and general concept inclusions and the *RBox* \mathcal{R} contains finitely many role inclusions. Such an ontology is an \mathcal{ELH}_{R^+} -*ontology* if \mathcal{R} contains only transitivity or role

hierarchy axioms, and an \mathcal{EL} -ontology if \mathcal{R} is empty. An interpretation is a *model* of an ontology if it satisfies all its axioms.

A TBox \mathcal{T} is an *acyclic TBox* if it contains only concept definitions such that no concept name occurs more than once on the left-hand side of a definition in \mathcal{T} and there are no cyclic dependencies between its concept definitions. To be more precise, we say that the concept name A *directly depends on* the concept name B in a TBox \mathcal{T} if \mathcal{T} contains a concept definition $A \equiv C$ and B occurs in C . Let *depends on* be the transitive closure of the relation *directly depends on*. A TBox \mathcal{T} is an *acyclic TBox* if there is no concept name A that depends on itself w.r.t. \mathcal{T} . Given an acyclic TBox \mathcal{T} , we call a concept name A a *defined concept* if it occurs as the left-side of a concept definition $A \equiv C$ in \mathcal{T} . All other concept names are called *primitive concepts*.

A *general TBox* is a TBox that contains only GCIs. Note that the notion of a general TBox indeed subsumes the notion of an acyclic TBox since the concept definition $A \equiv C$ can be expressed using the two GCIs $A \sqsubseteq C$ and $C \sqsubseteq A$.

2.3 Subsumption, Equivalence, and Role Hierarchy

A concept description C is *subsumed* by a concept description D w.r.t. an ontology \mathcal{O} (written $C \sqsubseteq_{\mathcal{O}} D$) if every model of \mathcal{O} satisfies the GCI $C \sqsubseteq D$. We say that C is *equivalent* to D w.r.t. \mathcal{O} ($C \equiv_{\mathcal{O}} D$) if $C \sqsubseteq_{\mathcal{O}} D$ and $D \sqsubseteq_{\mathcal{O}} C$. If \mathcal{O} is empty, we also write $C \sqsubseteq D$ and $C \equiv D$ instead of $C \sqsubseteq_{\mathcal{O}} D$ and $C \equiv_{\mathcal{O}} D$, respectively. As shown in [12, 3], subsumption w.r.t. \mathcal{EL}^+ -ontologies (and thus also w.r.t. \mathcal{ELH}_{R^+} - and \mathcal{EL} -ontologies) is decidable in polynomial time.

Since conjunction is interpreted as intersection, the concept descriptions $(C \sqcap D) \sqcap E$ and $C \sqcap (D \sqcap E)$ are always equivalent. Thus, we dispense with parentheses and write nested conjunctions in flat form $C_1 \sqcap \dots \sqcap C_n$. Nested existential restrictions $\exists r_1. \exists r_2. \dots \exists r_n. C$ will sometimes also be written as $\exists r_1 r_2 \dots r_n. C$, where $r_1 r_2 \dots r_n$ is viewed as a word over the alphabet of role names, i.e., an element of N_R^* .

Given a concept description C and an acyclic TBox \mathcal{T} , the description C can be *expanded* w.r.t. \mathcal{T} by replacing defined concepts by their definitions until no more defined concepts occur. This yields a concept description $C^{\mathcal{T}}$ that is equivalent to C w.r.t. \mathcal{T} and does not contain defined concepts. Expansion can be used to reduce subsumption w.r.t. an acyclic TBox to subsumption w.r.t. the empty TBox, but the expanded description can be exponential in the size of C and \mathcal{T} .

The *role hierarchy* induced by an ontology \mathcal{O} is a binary relation $\preceq_{\mathcal{O}}$ on N_R , which is defined as the reflexive-transitive closure of the relation $\{(r, s) \mid r \sqsubseteq s \in \mathcal{O}\}$. Using elementary reachability algorithms, the role hierarchy can be computed in polynomial time in the size of \mathcal{O} . It is easy to see that $r \preceq_{\mathcal{O}} s$ implies that $r^{\mathcal{I}} \subseteq s^{\mathcal{I}}$ for all models \mathcal{I} of \mathcal{O} .

2.4 Conservative Extensions

The following definition is useful to compare the expressiveness of ontologies, i.e., whether a certain ontology expresses more restrictions on interpretations than another one.

Definition 1. For an ontology \mathcal{O} , we denote by $sig(\mathcal{O}) \subseteq N_C \cup N_R$ the set of concept and role names occurring in \mathcal{O} . An ontology \mathcal{O}_2 is called a *conservative extension* of another ontology \mathcal{O}_1 if for all concept descriptions C, D built over the signature $sig(\mathcal{O}_1)$ we have $C \sqsubseteq_{\mathcal{O}_1} D$ iff $C \sqsubseteq_{\mathcal{O}_2} D$.

\mathcal{O}_2 is called a *model-theoretic conservative extension* of \mathcal{O}_1 if every model of \mathcal{O}_2 is a model of \mathcal{O}_1 and every model of \mathcal{O}_1 can be extended to a model of \mathcal{O}_2 by defining interpretations of additional concept and role names not occurring in \mathcal{O}_1 .

It is easy to prove that every model-theoretic conservative extension is also a conservative extension.

Intuitively, an ontology is a conservative extension of another ontology if both give the same answers to questions of the form “Does $C \sqsubseteq_{\mathcal{O}} D$ hold?”. In this case, a user can use them interchangeably when reasoning about a domain. This notion was introduced in [19] to detect whether changes to an ontology change its behavior w.r.t. subsumption reasoning. Such changes include, e.g., importing of other ontologies or adding new axioms.

For example, consider an ontology $\mathcal{O} = (\mathcal{T}, \mathcal{R})$, where \mathcal{T} is an acyclic TBox. By replacing every concept definition $A \equiv C$ by the GCIs $A \sqsubseteq C$ and $C \sqsubseteq A$, we obtain a general TBox. The resulting ontology is a conservative extension of \mathcal{O} .

2.5 Flat Ontologies

To simplify definitions and proofs, it is often convenient to normalize the ontology appropriately. To introduce this normal form, we need the notion of an atom.

An *atom* is a concept name or an existential restriction. Thus, every concept description C is a conjunction of atoms or \top . We call the atoms in this conjunction the *top-level atoms* of C . An atom is called *flat* if it is a concept name or an existential restriction of the form $\exists r.A$ for a concept name A . A GCI is called *flat* if it is of the form $C_1 \sqcap \dots \sqcap C_n \sqsubseteq D$ for flat atoms C_1, \dots, C_n, D with $n \geq 0$. If $n = 0$, then the left-hand side of the GCI is the empty conjunction, which is \top .

A *flat ontology* $\mathcal{O} = (\mathcal{T}, \mathcal{R})$ is an ontology in which \mathcal{T} contains only flat GCIs. To flatten \mathcal{O} , we first transform all concept definitions in \mathcal{T} into GCIs and then employ the procedure described in [4]. This procedure uses normalization rules to transform all GCIs in \mathcal{T} into one of the forms $A \sqsubseteq B$, $A_1 \sqcap A_2 \sqsubseteq B$, $A \sqsubseteq \exists r.B$, or $\exists r.A \sqsubseteq B$, where A, A_1, A_2, B are concept names or \top . These are either already

flat or can easily be transformed into flat GCIs: Axioms with \top on the right-hand side are true in all interpretations and can therefore simply be removed. We can further replace \top inside existential restrictions by a new concept name A_\top and introduce the GCI $\top \sqsubseteq A_\top$.

The transformation rules are the following:

- $\widehat{C} \sqcap D \rho E \longrightarrow \{A \equiv \widehat{C}, A \sqcap D \rho E\}$
- $C \rho D \sqcap \widehat{E} \longrightarrow \{C \rho D \sqcap A, A \equiv \widehat{E}\}$
- $\exists r.\widehat{C} \rho D \longrightarrow \{A \equiv \widehat{C}, \exists r.A \rho D\}$
- $C \rho \exists r.\widehat{D} \longrightarrow \{C \rho \exists r.A, A \equiv \widehat{D}\}$

In these rules, C, D, E stand for arbitrary concept descriptions, $\widehat{C}, \widehat{D}, \widehat{E}$ are concept descriptions that are not concept names, $r \in N_R$, and $\rho \in \{\sqsubseteq, \equiv\}$. The concept name A is always a new concept name not occurring in \mathcal{O} . Applying a rule $G \longrightarrow \mathcal{S}$ to an ontology \mathcal{O} changes it to $(\mathcal{O} \setminus \{G\}) \cup \mathcal{S}$.

After exhaustively applying these four rules, the resulting TBox \mathcal{T}' consists of flat GCIs of the required form and additional flat concept definitions. The fact that for each definition a new concept name is used ensures that these definitions form an acyclic TBox. In particular, for each newly introduced concept name A we can find a unique concept description C_A occurring in the original TBox such that $A \equiv_{\mathcal{T}'} C_A$ holds. It remains to transform these definitions into GCIs: A definition $A \equiv A_1 \sqcap A_2$ is replaced by $A \sqsubseteq A_1, A \sqsubseteq A_2$, and $A_1 \sqcap A_2 \sqsubseteq A$, while any definition of the form $A \equiv \exists r.A'$ is replaced by $A \sqsubseteq \exists r.A'$ and $\exists r.A' \sqsubseteq A$.

Thus, we can transform every ontology $\mathcal{O} = (\mathcal{T}, \mathcal{R})$ into a flat ontology $\mathcal{O}' = (\mathcal{T}', \mathcal{R})$ that is a conservative extension of \mathcal{O} .

3 Subsumption w.r.t. \mathcal{EL}^+ -Ontologies

Subsumption w.r.t. \mathcal{EL}^+ -ontologies can be decided in polynomial time [4]. For the purposes of deciding unification, however, we do not simply want a decision procedure for subsumption, but are more interested in a characterization of subsumption that helps us to find unifiers. The following characterization of subsumption w.r.t. the empty ontology has proven useful for \mathcal{EL} -unification algorithms before.

Lemma 2 ([7]). *Let $A_1, \dots, A_k, B_1, \dots, B_l$ be concept names and $C = A_1 \sqcap \dots \sqcap A_k \sqcap \exists r_1.C_1 \sqcap \dots \sqcap \exists r_m.C_m$ and $D = B_1 \sqcap \dots \sqcap B_l \sqcap \exists s_1.D_1 \sqcap \dots \sqcap \exists s_n.D_n$ concept descriptions. Then $C \sqsubseteq D$ iff $\{B_1, \dots, B_l\} \subseteq \{A_1, \dots, A_k\}$ and for every $j \in \{1, \dots, n\}$ there exists an $i \in \{1, \dots, m\}$ such that $r_i = s_j$ and $C_i \sqsubseteq D_j$.*

Thus, an atom C is subsumed by an atom D (w.r.t. \emptyset) iff $C = D$ is a concept name or $C = \exists r.C'$ and $D = \exists r.D'$ for a role name r and $C' \sqsubseteq D'$.

Lemma 3. *Let C and D be two concept descriptions. Then $C \sqsubseteq D$ iff every top-level atom of D subsumes a top-level atom of C .*

In the presence of an \mathcal{EL}^+ -ontology $\mathcal{O} = (\mathcal{T}, \mathcal{R})$, however, this characterization does not hold anymore. The aim of this section is to provide a generalized characterization of subsumption that takes into account the ontology \mathcal{O} . It is based on a rewrite relation that uses axioms as rewrite rules from right to left.

3.1 Proving Subsumptions by Rewriting

Intuitively, an axiom of the form $C \sqsubseteq D \in \mathcal{O}$ is used to replace D by C and an axiom of the form $r_1 \circ \dots \circ r_n \sqsubseteq s \in \mathcal{O}$ to replace $\exists s.C$ by $\exists r_1 \dots r_n.C$. In order to deal with associativity, commutativity, and idempotency of conjunction, it is convenient to represent concept descriptions as sets of atoms rather than as conjunctions of atoms.

Given an \mathcal{EL} -concept description C , the *description set* $\mathfrak{s}(C)$ associated with C is defined by induction:

- $\mathfrak{s}(A) := \{A\}$ for $A \in N_C$ and $\mathfrak{s}(\top) := \emptyset$;
- $\mathfrak{s}(C \sqcap D) := \mathfrak{s}(C) \cup \mathfrak{s}(D)$ and $\mathfrak{s}(\exists r.C) := \{\exists r.\mathfrak{s}(C)\}$.

For example, if $C = A \sqcap \exists r.(A \sqcap \exists r.\top)$, then $\mathfrak{s}(C) = \{A, \exists r.\{A, \exists r.\emptyset\}\}$. Sometimes we may also write $\{A, \{B, C\}\}$ for the description set $\{A, B, C\}$. In this setting, an atom is either a concept name or an existential restriction of the form $\exists r.M$ for a description set M .

To uniquely define positions, we fix an arbitrary bijection π from the set of all atoms over the signature $N_C \cup N_R$ to \mathbb{N} . This mapping fixes the position of any atom in a description set, i.e., it defines its index. We define the set $\text{Pos}(M) \subseteq \mathbb{N}^*$ of (*set*) *positions* of the description set M as follows:

$$\text{Pos}(M) := \{\varepsilon\} \cup \bigcup_{\exists r.M' \in M} \{\pi(\exists r.M')\} \text{Pos}(M).$$

Every position in $p \in \text{Pos}(M)$ uniquely identifies a *subdescription* $M|_p$ of M as follows:

- If $p = \varepsilon$, then $M|_p := M$.
- If $p = \pi(\exists r.M')p'$ for some $\exists r.M' \in M$, then $M|_p := M'|_{p'}$.

In our example, we have three set positions, corresponding to the description sets $\{A, \exists r.\{A, \exists r.\emptyset\}\}$, $\{A, \exists r.\emptyset\}$, and \emptyset . The set position ε that corresponds to the whole set M is called the *root position*.

Our *rewrite rules* are of the form $Q \leftarrow P$, where Q, P are description sets. For a description set M , $p \in \text{Pos}(M)$, and description sets Q, P , we define the description set $M[Q \leftarrow P]_p$ as follows:

- If $p = \varepsilon$, then $M[Q \leftarrow P]_p := (M \setminus P) \cup Q$.
- If $p = \pi(\exists r.M')p'$ for some $\exists r.M' \in M$, then

$$M[Q \leftarrow P]_p := (M \setminus \{\exists r.M'\}) \cup \{\exists r.(M'[Q \leftarrow P]_{p'})\}.$$

Given an \mathcal{EL}^+ -ontology $\mathcal{O} = (\mathcal{T}, \mathcal{R})$, the corresponding rewrite system $R(\mathcal{O})$ consists of the following rules:

- *Concept inclusion* (\mathbf{R}_c): For every $C \sqsubseteq D \in \mathcal{T}$, $R(\mathcal{O})$ contains the rule

$$s(C) \leftarrow s(D).$$

- *Role inclusion* (\mathbf{R}_r): For every $r_1 \circ \dots \circ r_n \sqsubseteq s \in \mathcal{R}$ and every concept description C , $R(\mathcal{O})$ contains the rule

$$s(\exists r_1 \dots r_n.C) \leftarrow s(\exists s.C).$$

- *Monotonicity* (\mathbf{R}_m): For every atom D , $R(\mathcal{O})$ contains the rule

$$s(D) \leftarrow \emptyset.$$

Definition 4. Let N, M be description sets. We write $N \leftarrow_{\mathcal{O}} M$ if there is a rule $Q \leftarrow P$ of the form (\mathbf{R}_c) , (\mathbf{R}_r) , or (\mathbf{R}_m) and a position $p \in \text{Pos}(M)$ such that $P \subseteq M|_p$ and $N = M[Q \leftarrow P]_p$.

We write $N \leftarrow_{Q \leftarrow P} M$ instead of $N \leftarrow_{\mathcal{O}} M$ to explicitly say which rule was applied. The relation $\leftarrow_{\mathcal{O}}^*$ is defined as the reflexive, transitive closure of $\leftarrow_{\mathcal{O}}$, i.e., $N \leftarrow_{\mathcal{O}}^* M$ iff there is a chain

$$N = M_l \leftarrow_{\mathcal{O}} M_{l-1} \leftarrow_{\mathcal{O}} \dots \leftarrow_{\mathcal{O}} M_0 = M$$

of $l \geq 0$ rule applications. We call such a chain a *derivation of N from M w.r.t. \mathcal{O}* . A rewriting step in such a derivation is called a *root step* if it applies a rule of the form (\mathbf{R}_c) at the root position. We write $N \xrightarrow{(n)}_{\mathcal{O}} M$ to express that there is a derivation of N from M w.r.t. \mathcal{O} that uses *at most n root steps*.

For example, if \mathcal{O} contains the axioms $\top \sqsubseteq \exists r.B$ and $s \sqsubseteq r$, then the following is a derivation w.r.t. \mathcal{O} :

$$\{A, \exists s.\{A\}\} \leftarrow_{\mathcal{O}} \{A, \exists r.\{A\}\} \leftarrow_{\mathcal{O}} \{A, \exists r.\{A, \exists r.\{B\}\}\} \leftarrow_{\mathcal{O}} \{A, \exists r.\{A, \exists r.\emptyset\}\}$$

This is a derivation without a root step, which first applies a rule of the form (\mathbf{R}_m) , then one of the form (\mathbf{R}_c) (not at the root position), and finally one of the form (\mathbf{R}_r) . This shows $s(A \sqcap \exists s.A) \xleftarrow{(0)}_{\mathcal{O}} s(A \sqcap \exists r.(A \sqcap \exists r.\top))$.

The first step in the characterization of $\sqsubseteq_{\mathcal{O}}$ by $\xleftarrow{*}_{\mathcal{O}}$ is to show that $\xleftarrow{*}_{\mathcal{O}}$ has similar properties as $\sqsubseteq_{\mathcal{O}}$; in particular, that it is closed under existential restrictions and conjunctions as follows.

Lemma 5. *Let \mathcal{O} be an \mathcal{EL}^+ -ontology and $n, n_1, n_2 \in \mathbb{N}$.*

1. *If N, M are two description sets with $N \xleftarrow{(n)}_{\mathcal{O}} M$ and r is a role name, then $\{\exists r.N\} \xleftarrow{(0)}_{\mathcal{O}} \{\exists r.M\}$.*
2. *If N, M, S are description sets with $N \xleftarrow{(n)}_{\mathcal{O}} M$, then $N \cup S \xleftarrow{(n)}_{\mathcal{O}} M \cup S$.*
3. *If N_1, N_2, M_1, M_2 are description sets with $N_i \xleftarrow{(n_i)}_{\mathcal{O}} M_i$ for $i \in \{1, 2\}$, then $N_1 \cup N_2 \xleftarrow{(n_1+n_2)}_{\mathcal{O}} M_1 \cup M_2$.*

Proof.

1. We prove this by induction on the length of the derivation

$$N = M_l \leftarrow_{\mathcal{O}} \dots \leftarrow_{\mathcal{O}} M_0 = M.$$

If $l = 0$, then $N = M$ and $\{\exists r.N\} \xleftarrow{(0)}_{\mathcal{O}} \{\exists r.M\}$ by reflexivity of $\xleftarrow{*}_{\mathcal{O}}$. Assume now that the claim holds for all shorter derivations and consider the first rule application $M_1 \leftarrow_{\mathcal{O}} M_0$. The rest of the derivation has length $l - 1$ and induction yields that $\{\exists r.N\} \xleftarrow{(0)}_{\mathcal{O}} \{\exists r.M_1\}$.

Let p be the position used in the step $M_1 \leftarrow_{\mathcal{O}} M_0$. It is clear that we can rewrite $\{\exists r.M_0\}$ into $\{\exists r.M_1\}$ by using the same rule at position $\pi(\exists r.M_0)p$, which is not a root step. Thus, $\{\exists r.M_1\} \xleftarrow{(0)}_{\mathcal{O}} \{\exists r.M_0\} = \{\exists r.M\}$, which yields $\{\exists r.N\} \xleftarrow{(0)}_{\mathcal{O}} \{\exists r.M\}$.

2. We again use induction on the length of the derivation

$$N = M_l \leftarrow_{\mathcal{O}} \dots \leftarrow_{\mathcal{O}} M_0 = M.$$

If $l = 0$, then $N = M$ and $N \cup S \xleftarrow{(0)}_{\mathcal{O}} M \cup S$ by reflexivity of $\xleftarrow{*}_{\mathcal{O}}$. Assume now that the claim holds for all shorter derivations and consider the first rule application $M_1 \leftarrow_{Q \leftarrow P} M_0$ at position p .

- If $p = \varepsilon$, then $M_1 = (M_0 \setminus P) \cup Q$. If we apply the same rule to $M_0 \cup S$ at position ε , we arrive at the concept description

$$((M_0 \cup S) \setminus P) \cup Q = (M_0 \setminus P) \cup (S \setminus P) \cup Q = M_1 \cup (S \setminus P).$$

Thus, we have the derivation

$$M_1 \cup (S \setminus P) \xleftarrow{(i)}_{\mathcal{O}} M_0 \cup S,$$

where $i = 1$ in the case that (\mathbf{R}_c) was applied and $i = 0$ otherwise.

In order to arrive at $M_1 \cup S$, for each atom $A \in S \cap P$ we apply a rule $\{A\} \leftarrow \emptyset$ of the form (\mathbf{R}_m) at position ε , which yields

$$M_1 \cup S = M_1 \cup (S \setminus P) \cup (S \cap P) \xleftarrow{(0)}_{\mathcal{O}} M_1 \cup (S \setminus P) \xleftarrow{(i)}_{\mathcal{O}} M_0 \cup S.$$

Since $N \xleftarrow{(n-i)}_{\mathcal{O}} M_1$, induction yields $N \cup S \xleftarrow{(n)}_{\mathcal{O}} M \cup S$.

- If $p = \pi(\exists r.M')p'$ for an atom $\exists r.M' \in M_0$, then

$$M_1 = (M_0 \setminus \{\exists r.M'\}) \cup \{\exists r.M''\},$$

where $M'' := M'[Q \leftarrow P]_{p'}$. Applying the same rule at the same position to $M_0 \cup S$ yields the derivation

$$M_1 \cup (S \setminus \{\exists r.M'\}) \leftarrow_{\mathcal{O}} M_0 \cup S.$$

If $\exists r.M' \in S$, we can proceed as above to reintroduce $\exists r.M'$ by applying the rule $\{\exists r.M'\} \leftarrow \emptyset$ at position ε . Thus, we have $M_1 \cup S \xleftarrow{(0)}_{\mathcal{O}} M_0 \cup S$, and by induction $N \cup S \xleftarrow{(n)}_{\mathcal{O}} M \cup S$.

3. We have $N_1 \cup N_2 \xleftarrow{(n_1)}_{\mathcal{O}} M_1 \cup N_2 \xleftarrow{(n_2)}_{\mathcal{O}} M_1 \cup M_2$ by 2. from above. \square

With the help of this lemma, we can now show that $\xleftarrow{*}_{\mathcal{O}}$ characterizes $\sqsubseteq_{\mathcal{O}}$ as follows.

Theorem 6. *Let \mathcal{O} be an \mathcal{EL}^+ -ontology and C, D be two \mathcal{EL} -concept descriptions. Then $C \sqsubseteq_{\mathcal{O}} D$ iff $\mathfrak{s}(C) \xleftarrow{*}_{\mathcal{O}} \mathfrak{s}(D)$.*

Proof. In order to show that $\mathfrak{s}(C) \xleftarrow{*}_{\mathcal{O}} \mathfrak{s}(D)$ implies $C \sqsubseteq_{\mathcal{O}} D$, it suffices to consider the case $\mathfrak{s}(C) \leftarrow_{\mathcal{O}} \mathfrak{s}(D)$ since the relation $\sqsubseteq_{\mathcal{O}}$ is reflexive and transitive. Let $N := \mathfrak{s}(C)$, $M := \mathfrak{s}(D)$, $Q \leftarrow P$ be a rule of the form (\mathbf{R}_c) , (\mathbf{R}_r) , or (\mathbf{R}_m) , and $p \in \text{Pos}(M)$ such that $P \subseteq M|_p$, and $N = M[Q \leftarrow P]_p$. We show by induction on the length of p that this implies $C \sqsubseteq_{\mathcal{O}} D$.

- If $p = \varepsilon$, then $N = (M \setminus P) \cup Q$. Let E, F, G denote the concept descriptions corresponding to $Q, P, M \setminus P$, respectively, i.e., $Q = \mathfrak{s}(E)$, $P = \mathfrak{s}(F)$, and $M \setminus P = \mathfrak{s}(G)$. Since the rules were chosen such that $E \sqsubseteq_{\mathcal{O}} F$, we clearly have

$$C \equiv G \sqcap E \sqsubseteq_{\mathcal{O}} G \sqcap F \equiv D$$

by the definition of $\sqsubseteq_{\mathcal{O}}$.

- If $p = \pi(\exists r.M')p'$ for some $\exists r.M' \in M$, then $N = (M \setminus \{\exists r.M'\}) \cup \{\exists r.M''\}$ and $M'' \leftarrow_{\mathcal{O}} M'$, where the replacement is located at p' . By induction, we have $D'' \sqsubseteq_{\mathcal{O}} D'$, where $M'' = \mathfrak{s}(D'')$ and $M' = \mathfrak{s}(D')$, which implies that $\exists r.D'' \sqsubseteq_{\mathcal{O}} \exists r.D'$. Thus, $C \sqsubseteq_{\mathcal{O}} D$ can be shown as above.

Conversely, assume that $\mathfrak{s}(C) \leftarrow_{\mathcal{O}}^* \mathfrak{s}(D)$ does not hold. We construct a canonical model \mathcal{I} of \mathcal{O} with $C^{\mathcal{I}} \not\sqsubseteq D^{\mathcal{I}}$. The domain of \mathcal{I} is the set \mathfrak{S} of all description sets over the signature $N_C \cup N_R$. For every concept name A , we define

$$A^{\mathcal{I}} := \{N \in \mathfrak{S} \mid N \leftarrow_{\mathcal{O}}^* \mathfrak{s}(A)\},$$

and for every role name r , we set

$$r^{\mathcal{I}} := \{(N, M) \in \mathfrak{S}^2 \mid N \leftarrow_{\mathcal{O}}^* \{\exists r.M\}\}.$$

We show that the equality $C'^{\mathcal{I}} = \{N \in \mathfrak{S} \mid N \leftarrow_{\mathcal{O}}^* \mathfrak{s}(C')\}$ holds for all \mathcal{EL} -concept descriptions C' by induction on the structure of C' .

If C' is a concept name, then the claim holds by definition of \mathcal{I} . If $C' = \top$, then $\mathfrak{s}(C') = \emptyset$ and it is clear that any description set can be produced from \emptyset by repeated application of rules of the form (\mathbf{R}_m) . Thus, $C'^{\mathcal{I}} = \mathfrak{S} = \{N \in \mathfrak{S} \mid N \leftarrow_{\mathcal{O}}^* \mathfrak{s}(C')\}$.

Let now $C' = \exists r.C''$ and assume that $C''^{\mathcal{I}} = \{N \in \mathfrak{S} \mid N \leftarrow_{\mathcal{O}}^* \mathfrak{s}(C'')\}$ holds. Thus, for every $N \in C'^{\mathcal{I}}$, by definition of $r^{\mathcal{I}}$ there is $M \in \mathfrak{S}$ such that $N \leftarrow_{\mathcal{O}}^* \{\exists r.M\}$ and $M \leftarrow_{\mathcal{O}}^* \mathfrak{s}(C'')$. By Lemma 5, this implies that $N \leftarrow_{\mathcal{O}}^* \{\exists r.M\} \leftarrow_{\mathcal{O}}^* \{\exists r.\mathfrak{s}(C'')\} = \mathfrak{s}(C')$. On the other hand, if $N \leftarrow_{\mathcal{O}}^* \mathfrak{s}(C') = \{\exists r.\mathfrak{s}(C'')\}$, then $(N, \mathfrak{s}(C'')) \in r^{\mathcal{I}}$. Furthermore, we have $\mathfrak{s}(C'') \in C''^{\mathcal{I}}$ by reflexivity of $\leftarrow_{\mathcal{O}}^*$, and thus $N \in (\exists r.C'')^{\mathcal{I}} = C'^{\mathcal{I}}$.

Consider now the remaining case that $C' = C_1 \sqcap C_2$ and assume that $C_i^{\mathcal{I}} = \{N \in \mathfrak{S} \mid N \leftarrow_{\mathcal{O}}^* \mathfrak{s}(C_i)\}$ for $i = 1, 2$. If $N \in C'^{\mathcal{I}} = C_1^{\mathcal{I}} \cap C_2^{\mathcal{I}}$, this implies that $N \leftarrow_{\mathcal{O}}^* \mathfrak{s}(C_1)$ and $N \leftarrow_{\mathcal{O}}^* \mathfrak{s}(C_2)$ hold. Since $\mathfrak{s}(C') = \mathfrak{s}(C_1) \cup \mathfrak{s}(C_2)$, Lemma 5 yields $N \leftarrow_{\mathcal{O}}^* \mathfrak{s}(C')$. On the other hand, if $N \leftarrow_{\mathcal{O}}^* \mathfrak{s}(C') = \mathfrak{s}(C_1) \cup \mathfrak{s}(C_2)$, then we can derive N from both $\mathfrak{s}(C_1)$ and $\mathfrak{s}(C_2)$ by adding repeated applications of rules of the form (\mathbf{R}_m) at position ε to the right-hand side of this derivation. This implies that $N \in C_1^{\mathcal{I}} \cap C_2^{\mathcal{I}} = C'^{\mathcal{I}}$.

We now use this to show that \mathcal{I} is actually a model of \mathcal{T} . For every GCI $E \sqsubseteq F$ in \mathcal{T} we have $\mathfrak{s}(E) \leftarrow_{\mathcal{O}} \mathfrak{s}(F)$, and thus $N \leftarrow_{\mathcal{O}}^* \mathfrak{s}(E)$ implies $N \leftarrow_{\mathcal{O}}^* \mathfrak{s}(F)$ for

all $N \in \mathfrak{S}$. Similarly, \mathcal{I} satisfies every role inclusion $r_1 \circ \dots \circ r_n \sqsubseteq s \in \mathcal{R}$ since whenever $N_{i-1} \xleftarrow{*}_{\mathcal{O}} \{\exists r_i.N_i\}$ holds for description sets N_0, \dots, N_n and all $i \in \{1, \dots, n\}$, then we have $N_0 \xleftarrow{*}_{\mathcal{O}} \{\exists r_1.\{\dots \{\exists r_n.N_n\}\dots\}\} \xleftarrow{\mathcal{O}} \{\exists s.N_n\}$ by Lemma 5.

Finally, we know that $\mathfrak{s}(C) \in C^{\mathcal{I}}$ since $\xleftarrow{*}_{\mathcal{O}}$ is reflexive, but $\mathfrak{s}(C) \notin D^{\mathcal{I}}$ by assumption. Thus, $C \not\sqsubseteq_{\mathcal{O}} D$. \square

We now show that we can restrict derivations to use at most $|\mathcal{T}|$ root steps, where $|\mathcal{T}|$ denotes the cardinality of the TBox \mathcal{T} of the \mathcal{EL}^+ -ontology $\mathcal{O} = (\mathcal{T}, \mathcal{R})$. This means that we need to apply each GCI of the ontology at most once at the root position ε .

Lemma 7. *Let $\mathcal{O} = (\mathcal{T}, \mathcal{R})$ be an \mathcal{EL}^+ -ontology and N, M be two description sets. Then $N \xleftarrow{*}_{\mathcal{O}} M$ iff $N \xleftarrow{(|\mathcal{T}|)}_{\mathcal{O}} M$.*

Proof. Obviously, $N \xleftarrow{(|\mathcal{T}|)}_{\mathcal{O}} M$ implies $N \xleftarrow{*}_{\mathcal{O}} M$. Consider now a derivation

$$N = M_l \xleftarrow{R_{l-1}} M_{l-1} \xleftarrow{R_{l-2}} \dots \xleftarrow{R_0} M_0 = M$$

with the least number of root steps and assume that this number is greater than $|\mathcal{T}|$. Then there must be a GCI $E \sqsubseteq F$ in \mathcal{T} that is applied twice at the root position. More precisely, there are two indices $j, j' \in \{0, \dots, l-1\}$ with $j < j'$ such that R_j and $R_{j'}$ are equal to $\mathfrak{s}(E) \leftarrow \mathfrak{s}(F)$ and are applied at position ε .

Let $\mathfrak{s}(E) = \{A_1, \dots, A_k\}$. We replace the root step $M_{j+1} \xleftarrow{R_j} M_j$ by the k rule applications

$$M'_{j+1} \xleftarrow{\{A_k\} \leftarrow \emptyset} \dots \xleftarrow{\{A_1\} \leftarrow \emptyset} M_j$$

of the form (\mathbf{R}_m) at position ε . We know that $M_{j+1} = (M_j \setminus \mathfrak{s}(F)) \cup \mathfrak{s}(E)$ and $M'_{j+1} = M_j \cup \{A_1, \dots, A_k\} = M_j \cup \mathfrak{s}(E)$. Since $\mathfrak{s}(F) \subseteq M_j$, this implies that $M'_{j+1} = M_{j+1} \cup \mathfrak{s}(F)$.

If m is the number of root steps in the derivation $M_{j'} \xleftarrow{R_{j'-1}} \dots \xleftarrow{R_{j+1}} M_{j+1}$, then by Lemma 5, we also have $M_{j'} \cup \mathfrak{s}(F) \xleftarrow{(m)}_{\mathcal{O}} M_{j+1} \cup \mathfrak{s}(F)$. Furthermore, since $R_{j'} = \mathfrak{s}(E) \leftarrow \mathfrak{s}(F)$, we have $\mathfrak{s}(F) \subseteq M_{j'}$, and thus $M_{j'} \cup \mathfrak{s}(F) = M_{j'}$. To sum up, there is a derivation

$$\begin{aligned} M_l &\xleftarrow{R_{l-1}} \dots \xleftarrow{R_{j'}} M_{j'} \\ &= M_{j'} \cup \mathfrak{s}(F) \xleftarrow{(m)}_{\mathcal{O}} M_{j+1} \cup \mathfrak{s}(F) \xleftarrow{(0)}_{\mathcal{O}} M_j \xleftarrow{R_{j-1}} \dots \xleftarrow{R_0} M_0 \end{aligned}$$

of $N = M_l$ from $M = M_0$ that uses fewer root steps than the original derivation, which contradicts the assumption. \square

Corollary 8. *Let $\mathcal{O} = (\mathcal{T}, \mathcal{R})$ be an \mathcal{EL}^+ -ontology and C, D be two \mathcal{EL} -concept descriptions. Then $C \sqsubseteq_{\mathcal{O}} D$ iff $\mathfrak{s}(C) \xleftarrow{(|\mathcal{T}|)}_{\mathcal{O}} \mathfrak{s}(D)$.*

3.2 A Structural Characterization of Subsumption in the Description Logic \mathcal{ELH}_{R^+}

Our translation of unification problems into propositional satisfiability problems depends on a structural characterization of subsumption, which we can unfortunately only show for \mathcal{ELH}_{R^+} -ontologies. Throughout this subsection, we assume that \mathcal{O} is a flat \mathcal{ELH}_{R^+} -ontology. We say that r is *transitive* if $r \circ r \sqsubseteq r$ belongs to \mathcal{O} .

Definition 9. Let C, D be atoms. We say that C is *structurally subsumed* by D w.r.t. \mathcal{O} ($C \sqsubseteq_{\mathcal{O}}^s D$) iff

- $C = D$ is a concept name,
- $C = \exists r.C'$, $D = \exists s.D'$, $C' \sqsubseteq_{\mathcal{O}} D'$, and $r \sqsubseteq s$, or
- $C = \exists r.C'$, $D = \exists s.D'$, and $C' \sqsubseteq_{\mathcal{O}} \exists t.D'$ for a transitive role t with $r \sqsubseteq_{\mathcal{O}} t \sqsubseteq_{\mathcal{O}} s$.

On the one hand, structural subsumption is a stronger property than $C \sqsubseteq_{\mathcal{O}} D$ since it requires the atoms C and D to have “compatible” top-level structures. On the other hand, it is weaker than subsumption \sqsubseteq w.r.t. the empty ontology, i.e., whenever $C \sqsubseteq D$ holds for two atoms C and D , then $C \sqsubseteq_{\mathcal{O}}^s D$, but not necessarily vice versa. If $\mathcal{O} = \emptyset$, then the three relations \sqsubseteq , $\sqsubseteq_{\mathcal{O}}^s$, $\sqsubseteq_{\mathcal{O}}$ coincide. Like \sqsubseteq and $\sqsubseteq_{\mathcal{O}}$, $\sqsubseteq_{\mathcal{O}}^s$ is reflexive, transitive, and closed under applying existential restrictions.

Lemma 10. Let C, D, E be atoms and r, s role names.

1. If $C \sqsubseteq D$, then $C \sqsubseteq_{\mathcal{O}}^s D$.
2. If $C \sqsubseteq_{\mathcal{O}}^s D$, then $\mathfrak{s}(C) \xleftarrow{(0)}_{\mathcal{O}} \mathfrak{s}(D)$, and thus $C \sqsubseteq_{\mathcal{O}} D$.
3. $C \sqsubseteq_{\mathcal{O}}^s C$.
4. If $C \sqsubseteq_{\mathcal{O}}^s D$ and $D \sqsubseteq_{\mathcal{O}}^s E$, then $C \sqsubseteq_{\mathcal{O}}^s E$.
5. If $C \sqsubseteq_{\mathcal{O}}^s D$ and $r \sqsubseteq_{\mathcal{O}} s$, then $\exists r.C \sqsubseteq_{\mathcal{O}}^s \exists s.D$.

Proof.

1. This follows from Lemma 2 and the fact that $\sqsubseteq_{\mathcal{O}}$ is reflexive.
2. If $C = D$ is a concept name, then obviously $C \xleftarrow{*}_{\mathcal{O}} D$ can be shown without any rewrite steps. Let now $C = \exists r.C'$ and $D = \exists s.D'$. If $C' \sqsubseteq_{\mathcal{O}} D'$ and $r \sqsubseteq_{\mathcal{O}} s$, then $\mathfrak{s}(C') \xleftarrow{*}_{\mathcal{O}} \mathfrak{s}(D')$. By Lemma 5, we have the derivation

$\{\exists r.s(C')\} \xleftarrow{(0)}_{\mathcal{O}} \{\exists s.s(C')\} \xleftarrow{(0)}_{\mathcal{O}} \{\exists s.s(D')\}$, which contains no root steps. If $C' \sqsubseteq_{\mathcal{O}} \exists t.D'$, t is transitive, and $r \trianglelefteq_{\mathcal{O}} t \trianglelefteq_{\mathcal{O}} s$, then $s(C') \xleftarrow{*}_{\mathcal{O}} \{\exists t.s(D')\}$. Again, Lemma 5 yields the derivation $\{\exists r.s(C')\} \xleftarrow{(0)}_{\mathcal{O}} \{\exists t.s(C')\} \xleftarrow{(0)}_{\mathcal{O}} \{\exists tt.s(D')\} \xleftarrow{\mathcal{O}} \{\exists t.s(D')\} \xleftarrow{(0)}_{\mathcal{O}} \{\exists s.s(D')\}$ without root steps.

3. This follows from claim 1. since $C \sqsubseteq C$ holds.
4. If $C = D$ is a concept name, then by $D \sqsubseteq_{\mathcal{O}}^s E$ also E must be the same concept name. Let now $C = \exists r.C'$, $D = \exists s.D'$, and $E = \exists t.E'$. If the second condition holds for C' and D' or for D' and E' , then the claim can easily be shown using transitivity and closure under existential restrictions of $\sqsubseteq_{\mathcal{O}}$. If we have two transitive roles s', t' with $r \trianglelefteq_{\mathcal{O}} s' \trianglelefteq_{\mathcal{O}} s \trianglelefteq_{\mathcal{O}} t' \trianglelefteq_{\mathcal{O}} t$, $C' \sqsubseteq_{\mathcal{O}} \exists s'.D'$, and $D' \sqsubseteq_{\mathcal{O}} \exists t'.E'$, then in particular $r \trianglelefteq_{\mathcal{O}} t' \trianglelefteq_{\mathcal{O}} t$ and

$$C' \sqsubseteq_{\mathcal{O}} \exists s'.D' \sqsubseteq_{\mathcal{O}} \exists t'.D' \sqsubseteq_{\mathcal{O}} \exists t't'.E' \sqsubseteq_{\mathcal{O}} \exists t'.E'.$$

5. If $C \sqsubseteq_{\mathcal{O}}^s D$ and $r \trianglelefteq_{\mathcal{O}} s$, then $C \sqsubseteq_{\mathcal{O}} D$ by claim 2., and thus $\exists r.C \sqsubseteq_{\mathcal{O}}^s \exists s.D$ since the second condition is satisfied. \square

Using the connection between subsumption and rewriting stated in Theorem 6, we can now prove a characterization of subsumption in the presence of an \mathcal{ELH}_{R^+} -ontology \mathcal{O} that expresses subsumption in terms of structural subsumptions and derivations w.r.t. $\xleftarrow{\mathcal{O}}$. Recall that all \mathcal{EL} -concept descriptions are conjunctions of atoms and that $C \sqsubseteq_{\mathcal{O}} D_1 \sqcap \dots \sqcap D_m$ iff for all $j \in \{1, \dots, m\}$ there is an l such that $s(C) \xleftarrow{(l)}_{\mathcal{O}} s(D_j)$.

Lemma 11. *Let $\mathcal{O} = (\mathcal{T}, \mathcal{R})$ be a flat \mathcal{ELH}_{R^+} -ontology, C_1, \dots, C_n, D be atoms, and $l \geq 0$. Then $s(C_1 \sqcap \dots \sqcap C_n) \xleftarrow{(l)}_{\mathcal{O}} s(D)$ iff there is*

1. an index $i \in \{1, \dots, n\}$ such that $C_i \sqsubseteq_{\mathcal{O}}^s D$; or
2. a GCI $A_1 \sqcap \dots \sqcap A_k \sqsubseteq B$ in \mathcal{T} such that
 - a) for every $\eta \in \{1, \dots, k\}$ we have $s(C_1 \sqcap \dots \sqcap C_n) \xleftarrow{(l-1)}_{\mathcal{O}} s(A_{\eta})$,
 - b) $s(C_1 \sqcap \dots \sqcap C_n) \xleftarrow{(l)}_{\mathcal{O}} s(B)$, and
 - c) $B \sqsubseteq_{\mathcal{O}}^s D$.

Proof. If $C_i \sqsubseteq_{\mathcal{O}}^s D$ holds for some $i \in \{1, \dots, n\}$, then by Lemma 10 we can construct a derivation

$$s(C_1 \sqcap \dots \sqcap C_n) \xleftarrow{(0)}_{\mathcal{O}} s(C_i) \xleftarrow{(0)}_{\mathcal{O}} s(D)$$

by applying several rules of the form (\mathbf{R}_m) to $\mathfrak{s}(C_i)$. This derivation contains $0 \leq l$ root steps. If $\mathfrak{s}(C_1 \sqcap \dots \sqcap C_n) \xleftarrow{\mathcal{O}}^{(l)} \mathfrak{s}(B)$ and $B \sqsubseteq_{\mathcal{O}}^s D$ for some atom B in \mathcal{T} , then by Lemma 10 we again have a derivation

$$\mathfrak{s}(C_1 \sqcap \dots \sqcap C_n) \xleftarrow{\mathcal{O}}^{(l)} \mathfrak{s}(B) \xleftarrow{\mathcal{O}}^{(0)} \mathfrak{s}(D)$$

using at most l root steps.

For the other direction, we show a more general claim: If $\mathfrak{s}(C_1 \sqcap \dots \sqcap C_n) \xleftarrow{\mathcal{O}}^{(l)} \mathfrak{s}(D_1 \sqcap \dots \sqcap D_m)$, where D_1, \dots, D_m are atoms, then for every D_j , $j \in \{1, \dots, m\}$, one of the conditions 1. or 2. is satisfied. Consider a derivation

$$\mathfrak{s}(C_1 \sqcap \dots \sqcap C_n) = M_k \leftarrow_{\mathcal{O}} \dots \leftarrow_{\mathcal{O}} M_0 = \mathfrak{s}(D_1 \sqcap \dots \sqcap D_m)$$

using at most l root steps. We prove the claim by induction on the length k of this derivation. For $k = 0$, we have $C_1 \sqcap \dots \sqcap C_n = D_1 \sqcap \dots \sqcap D_m$, and thus the first condition is satisfied for each of the atoms D_j by reflexivity of $\sqsubseteq_{\mathcal{O}}^s$.

Let now $k > 0$ and consider the rule $Q \leftarrow P$ used to derive M_1 from M_0 .

- If $Q \leftarrow P$ was applied at a position $p = \pi(D_j)p'$ for some $j \in \{1, \dots, m\}$, then $D_j = \exists r.E$ for some concept description E and $M_1 = (M_0 \setminus \mathfrak{s}(D_j)) \cup \{\exists r.\mathfrak{s}(E')\}$ for some concept description E' with $\mathfrak{s}(E') = \mathfrak{s}(E)[Q \leftarrow P]_{p'}$. By Theorem 6, $\mathfrak{s}(E') \leftarrow_{\mathcal{O}} \mathfrak{s}(E)$ implies $E' \sqsubseteq_{\mathcal{O}} E$, and thus we have $\exists r.E' \sqsubseteq_{\mathcal{O}}^s D_j$ by definition of $\sqsubseteq_{\mathcal{O}}^s$.

Consider now the remaining derivation $M_k \xleftarrow{\mathcal{O}}^* (M_0 \setminus \mathfrak{s}(D_j)) \cup \{\exists r.\mathfrak{s}(E')\}$ of length $k - 1$, which still uses at most l root steps. The claim for all atoms except D_j directly follows by induction. Additionally, one of the following cases must hold for $\exists r.E'$:

1. If $C_i \sqsubseteq_{\mathcal{O}}^s \exists r.E'$ for some $i \in \{1, \dots, n\}$, then $C_i \sqsubseteq_{\mathcal{O}}^s D_j$ by transitivity of $\sqsubseteq_{\mathcal{O}}^s$, i.e., Condition 1. is satisfied by D_j .
 2. If the second condition of the lemma applies, then Condition 2.c) for D_j again follows from transitivity of $\sqsubseteq_{\mathcal{O}}^s$. Conditions 2.a) and 2.b) are the same, regardless of whether $\exists r.E'$ or $D_j = \exists r.E$ is considered.
- If $Q \leftarrow P$ was applied at ε and is of the form (\mathbf{R}_m) , then $M_1 = M_0 \cup \mathfrak{s}(E) = \mathfrak{s}(D_1 \sqcap \dots \sqcap D_m \sqcap E)$ for some atom E . Thus, the claim for the atoms D_1, \dots, D_m directly follows by induction.
 - If $Q \leftarrow P$ was applied at ε and is of the form (\mathbf{R}_r) , then $M_1 = (M_0 \setminus \mathfrak{s}(D_j)) \cup \mathfrak{s}(E)$ for some D_j of the form $\exists r.F$ with $E = \exists s.F$ and $s \sqsubseteq r \in \mathcal{R}$ or $E = \exists rr.F$ and $r \circ r \sqsubseteq r \in \mathcal{R}$. In both cases, we have $E \sqsubseteq_{\mathcal{O}}^s D_j$ by Definition 9. The claim now follows by induction, exactly as in the case for $p = \pi(D_j)p'$.

- Finally, if this step is a root step, then $M_1 = (M_0 \setminus \mathfrak{s}(B)) \cup \mathfrak{s}(A_1 \sqcap \dots \sqcap A_k)$ for some flat GCI $A_1 \sqcap \dots \sqcap A_k \sqsubseteq B$ in \mathcal{T} . The claim for all atoms D_1, \dots, D_m except B follows by induction.

B itself obviously fulfills Condition 2.c) of the claim. We now show that $\mathfrak{s}(C_1 \sqcap \dots \sqcap C_n) \xleftarrow{(l-1)}_{\mathcal{O}} \mathfrak{s}(A_\eta)$ holds for every $\eta \in \{1, \dots, k\}$ by prepending appropriate rule applications of the form (\mathbf{R}_m) . We obtain a derivation

$$\mathfrak{s}(C_1 \sqcap \dots \sqcap C_n) = M_k \leftarrow_{\mathcal{O}} \dots \leftarrow_{\mathcal{O}} M_1 \xleftarrow{*(\mathbf{R}_m)} \mathfrak{s}(A_\eta),$$

in which the first root step of the original derivation was replaced by several rule applications of the form (\mathbf{R}_m) . Since the original derivation used at most l root steps, the constructed derivation uses at most $l - 1$ root steps. The derivation required for 2.b) can be constructed similarly. \square

This proof crucially depends on the transitivity of $\sqsubseteq_{\mathcal{O}}^{\mathfrak{s}}$. In fact, this is the main reason why we cannot deal with general \mathcal{EL}^+ -ontologies. While it is not hard to extend the definition of structural subsumption to more general kinds of ontologies, it is currently not clear how to do this such that the resulting relation is transitive; and without transitivity of structural subsumption, we cannot show a characterization analogous to the one in Lemma 11.

4 Unification

From now on, we assume that the set N_C is partitioned into *concept variables* (N_v) and *concept constants* (N_c). A *substitution* σ maps every variable to a concept description and can be extended to concept descriptions in the usual way. A concept description C is *ground* if it contains no variables and a substitution is *ground* if all concept descriptions in its range are ground. Similarly, an ontology is *ground* if it contains no variables.

Definition 12. Let \mathcal{O} be a ground ontology. A *unification problem* w.r.t. \mathcal{O} is a finite set $\Gamma = \{C_1 \sqsubseteq^? D_1, \dots, C_n \sqsubseteq^? D_n\}$ of subsumptions between \mathcal{EL} -concept descriptions. A substitution σ is a *unifier* of Γ w.r.t. \mathcal{O} if σ *solves* all the GCIs in Γ w.r.t. \mathcal{O} , i.e., if $\sigma(C_1) \sqsubseteq_{\mathcal{O}} \sigma(D_1), \dots, \sigma(C_n) \sqsubseteq_{\mathcal{O}} \sigma(D_n)$. We say that Γ is *unifiable* w.r.t. \mathcal{O} if it has a unifier w.r.t. \mathcal{O} .

We call Γ w.r.t. \mathcal{O} an \mathcal{EL} -, \mathcal{EL}^+ -, or \mathcal{ELH}_{R^+} -unification problem depending on whether and what kind of role inclusions are contained in \mathcal{O} .

Three remarks regarding this definition are in order. First, note that some of the previous papers on unification in DLs used equivalences $C \equiv^? D$ instead of subsumptions $C \sqsubseteq^? D$. This difference is, however, irrelevant since $C \equiv^? D$ can

be seen as a shorthand for the two subsumptions $C \sqsubseteq^? D$ and $D \sqsubseteq^? C$, and $C \sqsubseteq^? D$ has the same unifiers as $C \sqcap D \equiv^? C$.

Second, note that—as in [2]—we have restricted the background ontology \mathcal{O} to be ground. This is not without loss of generality. In fact, if \mathcal{O} contained variables, then we would need to apply the substitution also to its axioms, and instead of requiring $\sigma(C_i) \sqsubseteq_{\mathcal{O}} \sigma(D_i)$ we would thus need to require $\sigma(C_i) \sqsubseteq_{\sigma(\mathcal{O})} \sigma(D_i)$, which would change the nature of the problem considerably. The treatment of unification w.r.t. acyclic TBoxes in [7] actually considers a more general setting, where some of the primitive concepts occurring in the TBox may be variables. The restriction to ground general TBoxes is, however, appropriate for the application scenario sketched in the introduction. In this scenario, there is a fixed background ontology, which is extended with definitions of new concepts by several knowledge engineers. Unification w.r.t. the background ontology is used to check whether some of these new definitions actually are redundant, i.e., define the same intuitive concept. Here, some of the primitive concepts newly introduced by one knowledge engineer may be further defined by another one, but we assume that the knowledge engineers use the vocabulary from the background ontology unchanged, i.e., they define *new* concepts rather than adding definitions for concepts that already occur in the background ontology. An instance of this scenario can, e.g., be found in [13], where different extensions of SNOMED CT are checked for overlaps, albeit not by using unification, but by simply testing for equivalence.

Third, though we allow for arbitrary substitutions σ in the definition of a unifier, it is actually sufficient to consider ground substitutions such that all concept descriptions $\sigma(X)$ in the range of σ contain only concept and role names occurring in Γ or \mathcal{O} . It is an easy consequence of well-known results from unification theory [10] that Γ has a unifier w.r.t. \mathcal{O} iff it has such a ground unifier.

4.1 Unifiers versus Acyclic TBoxes

There is a close relationship between ground substitutions and acyclic TBoxes. Given a ground substitution σ , we can build the TBox $\mathcal{T}_\sigma := \{X \equiv \sigma(X) \mid X \in N_v\}$. Since σ is ground, this is indeed an acyclic TBox, and expansion w.r.t. \mathcal{T}_σ corresponds to applying σ , i.e., for every concept description C we have $\sigma(C) = C^{\mathcal{T}_\sigma}$. As an easy consequence of this observation we have for any ground ontology $\mathcal{O} = (\mathcal{T}, \mathcal{R})$:

$$\sigma(C) \sqsubseteq_{\mathcal{O}} \sigma(D) \text{ iff } C^{\mathcal{T}_\sigma} \sqsubseteq_{\mathcal{O}} D^{\mathcal{T}_\sigma} \text{ iff } C \sqsubseteq_{(\mathcal{T} \cup \mathcal{T}_\sigma, \mathcal{R})} D.$$

Conversely, any acyclic TBox \mathcal{S} whose defined concepts are the variables in N_v yields a ground substitution $\sigma_{\mathcal{S}}$, which is defined by setting $\sigma_{\mathcal{S}}(X) = X^{\mathcal{S}}$ for all variables X . Again, expansion w.r.t. the acyclic TBox corresponds to applying

the substitution, i.e., $C^{\mathcal{S}} = \sigma_{\mathcal{S}}(C)$, and thus

$$C \sqsubseteq_{(\mathcal{T} \cup \mathcal{S}, \mathcal{R})} D \text{ iff } C^{\mathcal{S}} \sqsubseteq_{\mathcal{O}} D^{\mathcal{S}} \text{ iff } \sigma_{\mathcal{S}}(C) \sqsubseteq_{\mathcal{O}} \sigma_{\mathcal{S}}(D).$$

This yields another view on what unification is trying to compute, and thus another potential application scenario: the extraction of concept definitions that imply a given set of GCIs w.r.t. a background ontology.

Proposition 13. *Let $\mathcal{O} = (\mathcal{T}, \mathcal{R})$ be a ground ontology and \mathcal{T}' an arbitrary general TBox. Then $\Gamma' := \{C \sqsubseteq^? D \mid C \sqsubseteq D \in \mathcal{T}'\}$ has a unifier w.r.t. \mathcal{O} iff there is an acyclic TBox \mathcal{S} whose defined concepts are the variables in N_v such that every GCI in \mathcal{T}' follows from $(\mathcal{T} \cup \mathcal{S}, \mathcal{R})$.*

4.2 Relationship to Equational Unification

Unification was originally not introduced for Description Logics, but for equational theories [10]. In [7] it was shown that equivalence and unification in \mathcal{EL} are the same as the word problem and unification, respectively, in the equational theory $SLmO$ of semilattices with monotone operators [21]. As argued in [2], unification in \mathcal{EL} w.r.t. a ground \mathcal{EL} -ontology corresponds to unification in $SLmO$ extended with a finite set of ground identities. We will see that, in contrast to GCIs, role inclusions add non-ground identities to $SLmO$.

The signature Σ_{SLmO} of this theory consists of a binary function symbol \wedge , a constant symbol 1 , and finitely many unary function symbols f_1, \dots, f_n . Terms can be built using these symbols and additional variable symbols and free constant symbols.

Definition 14. The equational theory of *semilattices with monotone operators* is defined by the following identities:

$$\begin{aligned} SLmO := & \{x \wedge (y \wedge z) = (x \wedge y) \wedge z, x \wedge y = y \wedge x, x \wedge x = x, x \wedge 1 = x\} \\ & \cup \{f_i(x \wedge y) \wedge f_i(y) = f_i(x \wedge y) \mid 1 \leq i \leq n\} \end{aligned}$$

Any \mathcal{EL} -concept description C using only the roles r_1, \dots, r_n can be translated into a term t_C over the signature Σ_{SLmO} by replacing each concept constant A by a free constant a , each concept variable X by a variable x , \top by 1 , \sqcap by \wedge , and $\exists r_i$ by f_i . For example, the \mathcal{EL} -concept description $C = A \sqcap \exists r_1. \top \sqcap \exists r_3. (X \sqcap B)$ is translated into $t_C = a \wedge f_1(1) \wedge f_3(x \wedge b)$. Conversely, any term t over the signature Σ_{SLmO} can be translated back into an \mathcal{EL} -concept description C_t . As shown in [21], the word problem in the theory $SLmO$ is the same as the equivalence problem for \mathcal{EL} -concept descriptions.

Lemma 15. *Let C, D be \mathcal{EL} -concept descriptions using only roles r_1, \dots, r_n . Then $C \equiv D$ iff $t_C =_{SLmO} t_D$.*

As an immediate consequence of this lemma, every \mathcal{EL} -unification problem can be translated into an $SLmO$ -unification problem that, modulo the translation between concept descriptions and terms, has the same unifiers.

Using this translation, any ground general TBox \mathcal{T} can be translated into a finite set $G_{\mathcal{T}}$ of ground identities by replacing each GCI $C \sqsubseteq D$ by the equation $t_C \wedge t_D = t_C$. Conversely, a set G of ground identities can be translated back into a ground general TBox \mathcal{T}_G by replacing every ground identity $s = t$ by the GCIs $C_s \sqsubseteq C_t$ and $C_t \sqsubseteq C_s$. Furthermore, a role inclusion $s_1 \circ \dots \circ s_m \sqsubseteq s_{m+1}$ can be expressed as a (non-ground) identity $f_1(\dots f_m(x)) = f_1(\dots f_m(x)) \wedge f_{m+1}(x)$. Thus, an RBox \mathcal{R} gives rise to a finite set $E_{\mathcal{R}}$ of additional identities. Lemma 15 can now be extended to account for an additional ground ontology [21].

Proposition 16. *Let $\mathcal{O} = (\mathcal{T}, \mathcal{R})$ be a ground ontology and C, D be \mathcal{EL} -concept descriptions using only roles r_1, \dots, r_n . Then $C \equiv_{\mathcal{O}} D$ iff $t_C =_{SLmO \cup E_{\mathcal{R}} \cup G_{\mathcal{T}}} t_D$.*

Unification in \mathcal{EL} w.r.t. a ground ontology, as introduced in Definition 12, thus corresponds to unification in $SLmO$ extended with additional identities. From a unification theory point of view, we are thus dealing with an instance of the following general question:

Problem. For which equational theories E does decidability and/or complexity transfer from E to all extensions of E by finite sets of identities (of a special form)?

The connection to equational unification also sheds some light on our decision to restrict unification to the case of ground ontologies. If we would lift this restriction, the background general TBox \mathcal{T} would contain variables, which are subject to substitution. For a substitution σ , we define $\sigma(\mathcal{T})$ to be the set of all GCIs $\sigma(C) \sqsubseteq \sigma(D)$ for all GCIs $C \sqsubseteq D$ in \mathcal{T} . Consider now the following generalization of Definition 12:²

Problem (\mathcal{EL} -unification w.r.t. a non-ground ontology). Given an ontology $\mathcal{O} = (\mathcal{T}, \mathcal{R})$ and an \mathcal{EL} -unification problem $\Gamma = \{C_1 \equiv^? D_1, \dots, C_n \equiv^? D_n\}$, is there a substitution σ that satisfies $\sigma(C_i) \equiv_{(\sigma(\mathcal{T}), \mathcal{R})} \sigma(D_i)$ for all $i \in \{1, \dots, n\}$?

According to the above translations, this is equivalent to finding a substitution σ with $\sigma(t_{C_i}) =_{SLmO \cup E_{\mathcal{R}} \cup \sigma(G_{\mathcal{T}})} \sigma(t_{D_i})$ for all $i \in \{1, \dots, n\}$, where the variables in $\sigma(G_{\mathcal{T}})$ are viewed as free constant symbols instead of proper (i.e., universally quantified) variables. This problem is related to the following problem [16, 15]:

Problem (Simultaneous rigid E -unification). Given finitely many equational theories E_1, \dots, E_n and terms $s_1, \dots, s_n, t_1, \dots, t_n$, is there a substitution σ that satisfies $\sigma(s_i) =_{\sigma(E_i)} \sigma(t_i)$ for all $i \in \{1, \dots, n\}$, where the variables in $\sigma(E_i)$ are treated as free constant symbols?

²We use equivalences rather than subsumptions in this definition to have a more direct connection to equational unification problems. As noted above, equivalences can be translated into subsumptions and vice versa.

Rigid E-unification is the special case where $n = 1$. In general, simultaneous rigid E -unification is undecidable [15], even in the case $n = 3$ with only 2 variables and ground terms s_1, s_2, s_3 [23]. For the case of only monadic function symbols, the problem is known to be PSPACE-hard [17], and in PSPACE if there is only one variable [18]. If there is only one variable, but arbitrary function symbols, then the problem is EXPTIME-complete [14]. The restricted problem of (non-simultaneous) rigid E -unification is decidable (more precisely, NP-complete) [16]. If there is only one variable, then the problem is P-complete [14].

Our problem is a generalization of rigid E -unification rather than simultaneous rigid E -unification since we use only one ontology \mathcal{O} rather than a different one for every equivalence. The main generalization is that we have $SLm\mathcal{O}$ as additional background theory. Whether the fact that we have several equivalences rather than a single one is relevant or not is not so clear. In fact, if \mathcal{O} is ground, then several equivalences can be encoded into a single one if sufficiently many *free* role names are available, i.e., role names that do not occur in \mathcal{O} . The following is an easy consequence of Lemma 11: if r_1, \dots, r_n are distinct free role names, then σ is a unifier of $\{C_1 \equiv^? D_1, \dots, C_n \equiv^? D_n\}$ w.r.t. \mathcal{O} iff it is a unifier of $\{\exists r_1.C_1 \sqcap \dots \sqcap \exists r_n.C_n \equiv^? \exists r_1.D_1 \sqcap \dots \sqcap \exists r_n.D_n\}$ w.r.t. \mathcal{O} . If \mathcal{O} is not ground, this trick does not necessarily work since, even if r_1, \dots, r_n are free w.r.t. $(\mathcal{T}, \mathcal{R})$, they may no longer be free w.r.t. $(\sigma(\mathcal{T}), \mathcal{R})$.

To sum up, \mathcal{EL} -unification w.r.t. non-ground ontologies is an instance of the following generalization of simultaneous rigid E -unification:

Problem (Simultaneous rigid E -unification with background theories). Consider finitely many equational theories $E_1, \dots, E_n, E'_1, \dots, E'_n$ and terms $s_1, \dots, s_n, t_1, \dots, t_n$. Is there a substitution σ that satisfies $\sigma(s_i) =_{E'_i \cup \sigma(E_i)} \sigma(t_i)$ for all $i \in \{1, \dots, n\}$, where the variables in $\sigma(E_i)$ are treated as free constant symbols?

The non-simultaneous version of this problem considers the case where $n = 1$. To the best of our knowledge, the problem of simultaneous or non-simultaneous rigid E -unification with background theory has not yet been considered in the literature, and it is probably quite hard to solve even in the non-simultaneous case. This is one of our reasons for restricting our attention to the case of a single ground ontology.

4.3 Flat Ontologies and Unification Problems

To simplify the technical development, it is convenient to flatten the ontology and the unification problem. Similar to flat ontologies, a unification problem Γ is called *flat* if all subsumptions in Γ are *flat*, i.e., of the form $C_1 \sqcap \dots \sqcap C_n \sqsubseteq^? D$ for $n \geq 0$ and flat atoms C_1, \dots, C_n, D .

Given an ontology \mathcal{O} and a unification problem Γ , we will first flatten \mathcal{O} as described in Section 2.5. Since the signature is changed by this process, this has

consequences for the unifiers: When looking for a unifier w.r.t. a given ontology one does not want this unifier to use auxiliary concept names introduced in a preprocessing step of the unification algorithm. The next lemma shows, however, that unifiability of a unification problem is not influenced by flattening the ontology. The proof of this lemma also shows how to remove unwanted auxiliary concept names from a unifier.

Lemma 17. *Let Γ be a unification problem, \mathcal{O} be an ontology, and \mathcal{O}' be the result of applying the normalization procedure from [4] to \mathcal{O} . Then Γ is unifiable w.r.t. \mathcal{O} iff it is unifiable w.r.t. \mathcal{O}' .*

Proof. Any unifier σ of Γ w.r.t. \mathcal{O} is also a unifier of Γ w.r.t. \mathcal{O}' since it is a conservative extension of \mathcal{O} . If, on the other hand, σ' is a unifier of Γ w.r.t. \mathcal{O}' , then its range may contain some of the newly introduced concept names. However, for each of these new concept names A there is a concept description C_A from \mathcal{O} such that $A \equiv_{\mathcal{O}'} C_A$. We now define the substitution σ by replacing all occurrences of the new concept names A by the concept descriptions C_A . Since equivalences are preserved under replacing subdescriptions by equivalent concept descriptions, σ is still a unifier of Γ w.r.t. \mathcal{O}' . Since it does not contain any concept names introduced by the normalization procedure, it is also a unifier of Γ w.r.t. \mathcal{O} over the original signature. \square

Furthermore, we also flatten the unification problem Γ by introducing new variables and equivalences, similar to the flattening procedure described in Section 2.5. This is not problematic, as any ground unifier w.r.t. of the flattened unification problem Γ' is immediately also a unifier of Γ and any ground unifier of Γ can easily be extended to a unifier of Γ' by defining the substitution of the auxiliary variables appropriately.

For this reason, we will assume in the following that all ontologies and unification problems are flat.

4.4 Cycle-Restricted Ontologies

The decidability and complexity results for unification w.r.t. \mathcal{EL} -ontologies in [2], and also the corresponding ones in the present report, only hold if the ontologies satisfy a restriction that prohibits certain cyclic subsumptions.

Definition 18. The \mathcal{EL}^+ -ontology \mathcal{O} is called *cycle-restricted* iff there is no nonempty word $w \in N_R^+$ and \mathcal{EL} -concept description C such that $C \sqsubseteq_{\mathcal{O}} \exists w.C$.

Note that, in contrast to acyclic TBoxes, cycle-restrictedness is not a syntactic condition on the form of the axioms in \mathcal{O} , but a semantic one on what follows from \mathcal{O} . In [1], cycle-restricted TBoxes were analyzed and it was shown that it can

be checked in polynomial time whether a given general TBox is cycle-restricted. However, this does not suffice to check cycle-restrictedness in the presence of an RBox since the role inclusions might introduce additional cycles, as the following example shows.

Example 19. The ontology (\mathcal{T}, \emptyset) with the general TBox

$$\mathcal{T} = \{A \sqsubseteq \exists r.B, \exists s.B \sqsubseteq \exists r.A\}$$

is cycle-restricted. However, the ontology $(\mathcal{T}, \mathcal{R})$ with $\mathcal{R} = \{r \sqsubseteq s\}$ is not, since, e.g., A is now subsumed by $\exists r.A$.

Although we cannot directly use the procedure from [1], we can use similar arguments to show that cycle-restrictedness of an \mathcal{ELH}_{R^+} -ontology can be checked in polynomial time. These arguments use the characterization of subsumption in Lemma 11. As a first step, we show that for flat \mathcal{ELH}_{R^+} -ontologies it suffices to consider cycles involving concept names and \top .

Lemma 20. *Let $\mathcal{O} = (\mathcal{T}, \mathcal{R})$ be a flat \mathcal{ELH}_{R^+} -ontology. Then \mathcal{O} is cycle-restricted iff there is no nonempty word $w \in N_R^+$ such that $\top \sqsubseteq_{\mathcal{O}} \exists w.\top$ or $A \sqsubseteq_{\mathcal{O}} \exists w.A$ for a concept name $A \in \text{sig}(\mathcal{O})$.*

Proof. The ‘only if’-direction is trivial. We prove the other direction by induction on the structure of C , which can be \top , a concept name, an existential restriction, or a conjunction of several atoms. Assume that $C \sqsubseteq_{\mathcal{O}} \exists w.C$ holds for some $w \in N_R^+$. If C is \top or a concept name in $\text{sig}(\mathcal{O})$, this immediately contradicts the assumption. By Lemma 11, one of the following cases must hold:

1. There is a top-level atom E of C such that $E \sqsubseteq_{\mathcal{O}}^s \exists w.C$. Note that in this case, C cannot be \top . We consider the remaining cases for the structure of C :
 - If C is a concept name that does not occur in \mathcal{O} , then $C = E \sqsubseteq_{\mathcal{O}}^s \exists w.C$ is impossible since w is not empty.
 - If $C = \exists r.D$ for a role name r and a concept description D , then we have $\exists r.D = C = E \sqsubseteq_{\mathcal{O}}^s \exists w.C = \exists wr.D$, and thus $w = sw'$, $r \trianglelefteq_{\mathcal{O}} s$, and either $D \sqsubseteq_{\mathcal{O}} \exists w'r.D$ or $D \sqsubseteq_{\mathcal{O}} \exists tw'r.D$ for some transitive role name t with $r \trianglelefteq_{\mathcal{O}} t \trianglelefteq_{\mathcal{O}} s$. This contradicts the induction hypothesis.
 - If $C = C_1 \sqcap \dots \sqcap C_n$, where C_1, \dots, C_n are atoms, then we have $C_i = E \sqsubseteq_{\mathcal{O}} \exists w.(C_1 \sqcap \dots \sqcap C_n) \sqsubseteq_{\mathcal{O}} \exists w.C_i$ for some $i \in \{1, \dots, n\}$, which again contradicts the induction hypothesis.
2. There is a GCI $A_1 \sqcap \dots \sqcap A_k \sqsubseteq \exists r.B$ in \mathcal{T} such that $C \sqsubseteq_{\mathcal{O}} A_1 \sqcap \dots \sqcap A_k$, $w = sw'$, $r \trianglelefteq_{\mathcal{O}} s$, and either $B \sqsubseteq_{\mathcal{O}} \exists w'.C$ or $B \sqsubseteq_{\mathcal{O}} \exists tw'.C$ for a transitive role name t with $r \trianglelefteq_{\mathcal{O}} t \trianglelefteq_{\mathcal{O}} s$. This implies that

$$B \sqsubseteq_{\mathcal{O}} \exists w'.C \sqsubseteq_{\mathcal{O}} \exists w'.(A_1 \sqcap \dots \sqcap A_k) \sqsubseteq_{\mathcal{O}} \exists w'r.B$$

or $B \sqsubseteq_{\mathcal{O}} \exists tw'.B$, respectively. Since \mathcal{T} is flat, B must be a concept name in $\text{sig}(\mathcal{O})$, and thus both subsumptions contradict the assumption. \square

For \mathcal{ELH}_{R^+} -ontologies, the condition in Definition 18 can now be tested by the following procedure, which is again based on Lemma 11.

Lemma 21. *Let \mathcal{O} be an \mathcal{ELH}_{R^+} -ontology. It can be decided in time polynomial in the size of \mathcal{O} whether \mathcal{O} is cycle-restricted or not.*

Proof. We first flatten $\mathcal{O} = (\mathcal{T}, \mathcal{R})$ as described in Section 2.5. The resulting ontology $\mathcal{O}' = (\mathcal{T}', \mathcal{R})$ has a larger signature than \mathcal{O} , but for each new concept name A there is a concept description C_A over the signature of the original ontology such that $A \equiv_{\mathcal{O}'} C_A$. It is clear that \mathcal{O}' is also an \mathcal{ELH}_{R^+} -ontology. Furthermore, we can show that \mathcal{O}' is cycle-restricted iff \mathcal{O} is. Assume first that \mathcal{O} is not cycle-restricted, i.e., there is a concept description C over $\text{sig}(\mathcal{O})$ and $w \in N_R^+$ such that $C \sqsubseteq_{\mathcal{O}} \exists w.C$. Since \mathcal{O}' is a conservative extension of \mathcal{O} , the same holds w.r.t. \mathcal{O}' , which shows that \mathcal{O}' is not cycle-restricted. On the other hand, if $C \sqsubseteq_{\mathcal{O}'} \exists w.C$ for $w \in N_R^+$ and a concept description C over $\text{sig}(\mathcal{O}')$, then we can replace each new concept name A by the equivalent C_A . The resulting concept description C' is built over $\text{sig}(\mathcal{O})$, and thus we have $C' \sqsubseteq_{\mathcal{O}} \exists w.C'$, i.e., \mathcal{O} is not cycle-restricted.

Thus, we can assume in the following that \mathcal{O} is flat. By Lemma 20, we only have to test for cycles involving concept names and \top . We first characterize such cycles in a convenient way. Let A be a concept name in $\text{sig}(\mathcal{O})$ or \top . By Lemma 11, $A \sqsubseteq_{\mathcal{O}} \exists rw'.A$ holds for some $w' \in N_R^*$ iff one of the two alternatives of this lemma holds. The first alternative cannot hold since $\exists rw'.A$ and A have an incompatible top-level structure – one is an existential restriction, the other is a concept name or \top . Thus, we have $A \sqsubseteq_{\mathcal{O}} \exists rw'.A$ iff there is a GCI $A'_1 \sqcap \dots \sqcap A'_k \sqsubseteq \exists s.B$ in \mathcal{T} such that $A \sqsubseteq_{\mathcal{O}} A'_1 \sqcap \dots \sqcap A'_k$, $s \sqsubseteq_{\mathcal{O}} r$, and either $B \sqsubseteq_{\mathcal{O}} \exists w'.A$ or $B \sqsubseteq_{\mathcal{O}} \exists tw'.A$ for a transitive role name t with $s \sqsubseteq_{\mathcal{O}} t \sqsubseteq_{\mathcal{O}} r$. Since \mathcal{T} is flat, B must be a concept name in $\text{sig}(\mathcal{O})$.

Thus, $A \sqsubseteq_{\mathcal{O}} \exists rw'.A$ implies $A \sqsubseteq_{\mathcal{O}} \exists s.B$ and $B \sqsubseteq_{\mathcal{O}} \exists w'.A$ or $B \sqsubseteq_{\mathcal{O}} \exists tw'.A$ for some concept name $B \in \text{sig}(\mathcal{O})$ and role names s, t . We can now apply the same argument to $B \sqsubseteq_{\mathcal{O}} \exists w'.A$ or $B \sqsubseteq_{\mathcal{O}} \exists tw'.A$ to derive the new subsumptions $B \sqsubseteq_{\mathcal{O}} \exists s_2.B_2$ and $B_2 \sqsubseteq_{\mathcal{O}} \exists t_2w'.A$ or $B_2 \sqsubseteq_{\mathcal{O}} \exists t_2w''.A$ or $B_2 \sqsubseteq_{\mathcal{O}} \exists w''.A$ for $w' = r'w''$ and some concept name $B_2 \in \text{sig}(\mathcal{O})$ and role names s_2, t_2 . We can continue to apply this argument indefinitely unless there are no more existential restrictions on the right-hand side of the subsumptions.

If this process stops, then we have constructed a sequence of subsumptions of the form $A \sqsubseteq_{\mathcal{O}} \exists s.B, B \sqsubseteq_{\mathcal{O}} \exists s_2.B_2, \dots, B_{n-1} \sqsubseteq_{\mathcal{O}} \exists s_n.B_n, B_n \sqsubseteq_{\mathcal{O}} A$ involving only A and concept and role names of $\text{sig}(\mathcal{O})$. If this process does not stop, then there is an infinite sequence $A \sqsubseteq_{\mathcal{O}} \exists s.B, B \sqsubseteq_{\mathcal{O}} \exists s_2.B_2, B_2 \sqsubseteq_{\mathcal{O}} \exists s_3.B_3, \dots$ of such subsumptions. Since \mathcal{O} is finite, we must have $B_i = B_j$ for some $j > i$.

Thus, in both cases we can find a finite sequence of subsumptions of the form $B_{k-1} \sqsubseteq_{\mathcal{O}} \exists s_k. B_k$ that starts and ends with the same concept name (or \top) and involves at least one role name.

Using the polynomial-time subsumption algorithm for \mathcal{EL}^+ , we can build a graph whose nodes are the elements for $N_C \cup \{\top\}$ and where there is an edge from A to B iff $A \sqsubseteq_{\mathcal{O}} \exists r. B$ for some $r \in N_R$. Then we can use standard reachability algorithms to check whether this graph contains a cycle of the above form. \square

We illustrate the procedure described in this proof on a simple example.

Example 22. Consider the general TBox $\{\exists r. A \sqsubseteq A, A \sqsubseteq \exists s. B\}$ and the RBox $\{s \sqsubseteq r\}$. The graph constructed in Lemma 21 has the tree nodes A , B , and \top . It contains s - and r -edges from A to B and from A to \top and ε -edges from A to \top and from B to \top . Since these edges form no cycles, the ontology is cycle-restricted.

The main reason why we need cycle-restrictedness of \mathcal{O} is that it ensures that a substitution always induces a strict partial order on the variables. To be more precise, assume that γ is a substitution. For $X, Y \in N_v$ we define

$$X >_{\gamma} Y \quad \text{iff} \quad \gamma(X) \sqsubseteq_{\mathcal{O}} \exists w. \gamma(Y) \text{ for some } w \in N_R^+.$$

Transitivity of $>_{\gamma}$ is an easy consequence of transitivity of subsumption, and cycle-restrictedness of \mathcal{O} yields irreflexivity of $>_{\gamma}$.

Lemma 23. *If \mathcal{O} is a cycle-restricted \mathcal{EL}^+ -ontology, then $>_{\gamma}$ is a strict partial order on N_v .*

5 Reduction to SAT

The main idea underlying the NP-membership results in [5] and [2] is to show that any \mathcal{EL} -unification problem that is unifiable w.r.t. the empty ontology and w.r.t. a cycle-restricted \mathcal{EL} -ontology, respectively, has a so-called local unifier. Here, we generalize the notion of a local unifier to the case of unification w.r.t. cycle-restricted \mathcal{ELH}_{R^+} -ontologies, but then go a significant step further. Instead of using an algorithm that “blindly” generates all local substitutions and then checks whether they are unifiers, we reduce the search for a local unifier to a propositional satisfiability problem.

5.1 Local Unifiers

Let Γ be a flat \mathcal{EL} -unification problem and $\mathcal{O} = (\mathcal{T}, \mathcal{R})$ be a flat, cycle-restricted \mathcal{ELH}_{R^+} -ontology. We denote by At the set of atoms occurring as subdescriptions

in subsumptions in Γ or axioms in \mathcal{O} and define

$$\mathbf{At}_{\text{tr}} := \mathbf{At} \cup \{\exists t.D' \mid \exists s.D' \in \mathbf{At}, t \trianglelefteq_{\mathcal{O}} s, t \text{ transitive}\}.$$

Furthermore, we define the set of *non-variable atoms* by $\mathbf{At}_{\text{nv}} := \mathbf{At}_{\text{tr}} \setminus N_v$. Though the elements of \mathbf{At}_{nv} cannot be variables, they may contain variables if they are of the form $\exists r.X$ for some role r and a variable X .

Let now S be an assignment function that maps every variable $X \in N_v$ to a set $S_X \subseteq \mathbf{At}_{\text{nv}}$. Every such assignment S induces a unique TBox

$$\mathcal{T}_S := \{X \equiv \prod_{D \in S_X} D \mid X \in N_v\}.$$

We call the assignment S *acyclic* if \mathcal{T}_S is acyclic. Thus, if S is acyclic, the TBox \mathcal{T}_S induces a unique substitution $\sigma_{\mathcal{T}_S}$. To simplify the notation, we write this substitution as σ_S . It is easy to see that this substitution satisfies

$$\sigma_S(X) = \prod_{D \in S_X} \sigma_S(D)$$

for all $X \in N_v$. We call a substitution σ *local* if it is of this form, i.e., if there is an acyclic assignment S such that $\sigma = \sigma_S$.

Thus, if we know that any solvable unification problem has a local unifier, then we can enumerate (or guess, in a nondeterministic machine) all local substitutions and then check whether any of them is a unifier. Thus, in general many substitutions will be generated that only in the subsequent check turn out not to be unifiers. In contrast, our SAT reduction will ensure that only unifiers are generated.

5.2 The Reduction

Here, we reduce unification in \mathcal{EL} w.r.t. cycle-restricted \mathcal{ELH}_{R^+} -ontologies to the satisfiability problem for propositional logic, which is NP-complete. This shows that this unification problem is in NP. But more importantly, it immediately allows us to apply highly optimized SAT-solvers for solving such unification problems.

As before, we assume that Γ is a flat \mathcal{EL} -unification problem and $\mathcal{O} = (\mathcal{T}, \mathcal{R})$ is a flat, cycle-restricted \mathcal{ELH}_{R^+} -ontology. We define the set

$$\text{Left} := \mathbf{At} \cup \{C_1 \sqcap \dots \sqcap C_n \mid C_1 \sqcap \dots \sqcap C_n \sqsubseteq^? D \in \Gamma \text{ for some } D \in \mathbf{At}\}$$

that contains all atoms of Γ and \mathcal{O} and all left-hand sides of subsumptions from Γ . For $L \in \text{Left}$ and $C \in \mathbf{At}$, we write “ $C \in L$ ” if C is a top-level atom of L .

The propositional variables we use for the reduction are of the form $[L \sqsubseteq D]^i$ for $L \in \text{Left}$, $D \in \text{At}_{\text{tr}}$, and $i \in \{0, \dots, |\mathcal{T}|\}$. The intuition behind these variables is that every satisfying valuation induces an acyclic assignment S such that the following holds for the induced substitution γ_S : $[L \sqsubseteq D]^i$ is evaluated to true iff $\mathfrak{s}(\gamma_S(L))$ can be derived from $\mathfrak{s}(\gamma_S(D))$ using at most i root steps, i.e., $\mathfrak{s}(\gamma_S(L)) \stackrel{(i)}{\leftarrow}_{\mathcal{O}} \mathfrak{s}(\gamma_S(D))$.

Additionally, we use the propositional variables $[X > Y]$ for $X, Y \in N_v$ to express the *depends on* relation between variables induced by the acyclic TBox \mathcal{T}_S that defines the desired local substitution.

The auxiliary function Dec is defined as follows for $C \in \text{At}$, $D \in \text{At}_{\text{tr}}$:

$$\text{Dec}(C \sqsubseteq D) = \begin{cases} \mathbf{1} & \text{if } C = D \\ [C \sqsubseteq D]^{|\mathcal{T}|} & \text{if } C \text{ and } D \text{ are ground} \\ \text{Trans}(C \sqsubseteq D) & \text{if } C = \exists r.C', D = \exists s.D', \text{ and } r \preceq_{\mathcal{O}} s, \\ [C \sqsubseteq D]^{|\mathcal{T}|} & \text{if } C \text{ is a variable} \\ \mathbf{0} & \text{otherwise} \end{cases}$$

$$\text{Trans}(C \sqsubseteq D) = [C' \sqsubseteq D']^{|\mathcal{T}|} \vee \bigvee_{\substack{t \text{ transitive} \\ r \preceq_{\mathcal{O}} t \preceq_{\mathcal{O}} s}} [C' \sqsubseteq \exists t.D']^{|\mathcal{T}|}.$$

Note that $C' \in \text{At}$ and $D', \exists t.D' \in \text{At}_{\text{tr}}$ by definition of At_{tr} and since Γ and \mathcal{O} are flat. Here, $\mathbf{0}$ and $\mathbf{1}$ are Boolean constants representing the truth values 0 (*false*) and 1 (*true*), respectively.

The unification problem will be reduced to satisfiability of the following set of propositional formulae. For simplicity, we do not use only clauses here. However, our formulae can be transformed into clausal form by introducing polynomially many auxiliary propositional variables and clauses.

Definition 24. Let Γ be a flat unification problem and $\mathcal{O} = (\mathcal{T}, \mathcal{R})$ be a flat, cycle-restricted \mathcal{ELH}_{R^+} -ontology. The set $C(\Gamma, \mathcal{O})$ contains the following propositional formulae:

- (I) *Translation of the subsumptions of Γ .* For every $L \sqsubseteq^? D$ in Γ , we introduce a clause asserting that this subsumption must hold:

$$\rightarrow [L \sqsubseteq D]^{|\mathcal{T}|}.$$

- (II) *Translation of the relevant properties of subsumption.*

- 1) For all ground atoms $C \in \text{At}$, $D \in \text{At}_{\text{tr}}$ and $i \in \{0, \dots, |\mathcal{T}|\}$ such that $C \not\sqsubseteq_{\mathcal{O}} D$ does not hold, we introduce a clause preventing this subsumption:

$$[C \sqsubseteq D]^i \rightarrow .$$

- 2) For every variable Y , $B \in \mathbf{At}_{\text{nv}}$, $i, j \in \{0, \dots, |\mathcal{T}|\}$, and $L \in \text{Left}$, we introduce the clause

$$[L \sqsubseteq Y]^i \wedge [Y \sqsubseteq B]^j \rightarrow [L \sqsubseteq B]^{\min\{|\mathcal{T}|, i+j\}}.$$

- 3) For every $L \in \text{Left} \setminus N_v$ and $D \in \mathbf{At}_{\text{tr}}$, we introduce the following formulae, depending on L and D :

- a) If D is a ground atom and L is not a ground atom, we introduce

$$[L \sqsubseteq D]^i \rightarrow \bigvee_{C \in L} \text{Dec}(C \sqsubseteq D) \vee \bigvee_{\substack{A_1 \sqcap \dots \sqcap A_k \sqsubseteq B \in \mathcal{T} \\ B \sqsubseteq_{\mathcal{O}} D}} ([L \sqsubseteq A_1]^{i-1} \wedge \dots \wedge [L \sqsubseteq A_k]^{i-1})$$

for all $i \in \{1, \dots, |\mathcal{T}|\}$ and

$$[L \sqsubseteq D]^0 \rightarrow \bigvee_{C \in L} \text{Dec}(C \sqsubseteq D).$$

- b) If D is a non-variable, non-ground atom, we introduce

$$[L \sqsubseteq D]^i \rightarrow \bigvee_{C \in L} \text{Dec}(C \sqsubseteq D) \vee \bigvee_{A \text{ atom of } \mathcal{T}} ([L \sqsubseteq A]^i \wedge \text{Dec}(A \sqsubseteq D))$$

for all $i \in \{1, \dots, |\mathcal{T}|\}$ and

$$[L \sqsubseteq D]^0 \rightarrow \bigvee_{C \in L} \text{Dec}(C \sqsubseteq D).$$

(III) *Translation of the relevant properties of $>$.*

- 1) Transitivity and irreflexivity of $>$ is expressed by the clauses

$$[X > X] \rightarrow \text{and } [X > Y] \wedge [Y > Z] \rightarrow [X > Z]$$

for all $X, Y, Z \in N_v$.

- 2) The connection between $>$ and \sqsubseteq is expressed using the clause

$$[X \sqsubseteq \exists r.Y]^i \rightarrow [X > Y]$$

for every $X, Y \in N_v$, $\exists r.Y \in \mathbf{At}_{\text{tr}}$, and $i \in \{0, \dots, |\mathcal{T}|\}$.

It is easy to see that the set $C(\Gamma, \mathcal{O})$ can be constructed in polynomial time in the size of Γ and \mathcal{O} . In particular, subsumptions $B \sqsubseteq_{\mathcal{O}} D$ between ground atoms B, D can be checked in polynomial time in the size of \mathcal{O} [4].

There are several differences between $C(\Gamma, \mathcal{O})$ and the clauses constructed in [6] to solve unification in \mathcal{EL} w.r.t. the empty ontology. First, the propositional variables employed in [6] are of the form $[C \not\sqsubseteq D]$ for atoms C, D of Γ , i.e., they stand for non-subsumption rather than subsumption. The use of single atoms C instead of whole right-hand sides L also leads to a different encoding of the subsumptions from Γ in part (I). The clauses in (III) are identical up to negation of the variable $[X \sqsubseteq \exists r.Y]^i$. But most importantly, in [6] the properties of subsumption expressed in (II) need only deal with subsumption w.r.t. the empty ontology (see Lemma 2), whereas here we have to take a cycle-restricted \mathcal{ELH}_{R^+} -ontology into account. We do this by expressing the characterization of subsumption given in Lemma 11. This is also the reason why the propositional variables $[L \sqsubseteq D]^i$ have an additional index i : in Lemma 11 we refer to the number of root steps in the derivation that shows the subsumption, and this needs to be modeled in our SAT reduction.

We now show that Γ is solvable w.r.t. \mathcal{O} iff $C(\Gamma, \mathcal{O})$ is satisfiable. The proof is divided into two parts that correspond to the following two subsections.

5.3 Soundness of the Reduction

Let τ be a valuation of the propositional variables that satisfies $C(\Gamma, \mathcal{O})$. We must show that then Γ has a unifier w.r.t. \mathcal{O} . To this purpose, we use τ to define an assignment S by

$$S_X := \{D \in \text{At}_{\text{nv}} \mid \exists i \in \{0, \dots, |\mathcal{T}|\} : \tau([X \sqsubseteq D]^i) = 1\}.$$

We first show the following connection between the variables $[X > Y]$ and the *depends on* relation induced by \mathcal{T}_S . This is similar to Lemma 3.5 of [6].

Lemma 25. *Let $X, Y \in N_v$.*

1. *If X depends on Y w.r.t. \mathcal{T}_S , then $\tau([X > Y]) = 1$.*
2. *The depends on relation is irreflexive, i.e., X cannot depend on itself.*

Proof.

1. If X *directly depends on* the variable Y , then Y appears in a non-variable atom of S_X . This atom must be of the form $\exists r.Y$. By the construction of S_X , $\exists r.Y \in S_X$ can only be the case if $\tau([X \sqsubseteq \exists r.Y]^i) = 1$ for some $i \in \{0, \dots, |\mathcal{T}|\}$. Since τ satisfies the clause $[X \sqsubseteq \exists r.Y]^i \rightarrow [X > Y]$ in (III)2), this implies $\tau([X > Y]) = 1$.

Since the transitivity clauses introduced in (III)1) are satisfied by τ , we also have that $\tau([X > Y]) = 1$ whenever X *depends on* the variable Y .

2. If X depends on itself, then $\tau([X > X]) = 1$ by the first part of this lemma. This is, however, impossible since τ satisfies the clause $[X > X] \rightarrow$. \square

The second part of this lemma shows that \mathcal{T}_S is acyclic. In the following, we denote by $>_S$ be the *depends on* relation on N_v induced by \mathcal{T}_S and by σ be the induced substitution. We will show that σ is a unifier of Γ w.r.t. \mathcal{O} .

As described in Lemma 23, the substitution σ induces a strict partial order $>_\sigma$ on the variables in N_v . We now extend this order to the set \mathbf{At} by setting $C >_\sigma D$ iff $\sigma(C) \sqsubseteq_{\mathcal{O}} \exists w.\sigma(D)$ for some $w \in N_R^+$. This relation is still transitive and irreflexive for the same reasons as before. Since \mathbf{At} is finite, $>_\sigma$ is also well-founded.

For $D \in \mathbf{At}_{\text{tr}}$, we define

$$\text{Var}(D) := \begin{cases} D & \text{if } D \in N_v \\ Y & \text{if } D = \exists r.Y \text{ for } Y \in N_v \text{ and } r \in N_R \\ \perp & \text{if } D \text{ is ground} \end{cases}$$

We extend $>_\sigma$ to the set $\mathbf{At} \cup \{\perp\}$ by defining \perp as the smallest element, i.e., we have $C >_\sigma \perp$ for all $C \in \mathbf{At}$.

Lemma 26. *If $\tau([C \sqsubseteq D]^i) = 1$ for $C \in \mathbf{At}$, $D \in \mathbf{At}_{\text{tr}}$, and $i \in \{0, \dots, |\mathcal{T}|\}$, then $\sigma(C) \sqsubseteq_{\mathcal{O}} \sigma(D)$.*

Proof. We prove the claim by induction on the lexicographic order on the tuples $(C, \text{Var}(D), i)$, where the first two components are compared using $>_\sigma$ and the third uses the usual order $>$ on natural numbers. The lexicographic product of these three well-founded orders is also well-founded and can thus be used for well-founded induction [9].

We make a case distinction depending on the form of D and consider first the case that D is a variable. Let $\sigma(B)$ be any top-level atom of $\sigma(D)$, i.e., $\tau([D \sqsubseteq B]^j) = 1$ for some $j \in \{0, \dots, |\mathcal{T}|\}$. By the formulae in (II)2), we have $\tau([C \sqsubseteq B]^k) = 1$ for $k = \min\{|\mathcal{T}|, i + j\}$. We also know that $C = C$ and $\text{Var}(D) = D >_\sigma \text{Var}(B)$ since $\sigma(D) \sqsubseteq_{\mathcal{O}} \sigma(B)$ and $B \in \mathbf{At}_{\text{nv}}$ by construction of σ . Thus, we can use induction to infer that $\sigma(C) \sqsubseteq_{\mathcal{O}} \sigma(B)$ holds, which implies that $\sigma(C) \sqsubseteq_{\mathcal{O}} \sigma(D)$.

If D is a ground atom, then we distinguish cases for C :

- If C is a variable, then $\sigma(C) \sqsubseteq_{\mathcal{O}} \sigma(D)$ holds by the construction of σ .
- If C is also ground, then $C \sqsubseteq_{\mathcal{O}} D$ must hold, since otherwise τ would violate the clause $[C \sqsubseteq D]^i \rightarrow$ in (II)1).
- If C is neither ground nor a variable, then it cannot be equal to D , and thus according to the formulae in (II)3a), we have one of the following cases:

- If $\text{Dec}(C \sqsubseteq D)$ is evaluated to 1 under τ , then $C = \exists r.C'$, $D = \exists s.D'$, $r \sqsubseteq s$, and either $\tau([C' \sqsubseteq D']^{|\mathcal{T}|}) = 1$ or $\tau([C' \sqsubseteq \exists t.D']^{|\mathcal{T}|}) = 1$ for a transitive role name t with $r \sqsubseteq_{\mathcal{O}} t \sqsubseteq_{\mathcal{O}} s$. We also know that $C >_{\sigma} C'$ since $\sigma(C) = \exists r.\sigma(C')$. By induction, we now have $\sigma(C') \sqsubseteq_{\mathcal{O}} D'$ or $\sigma(C') \sqsubseteq_{\mathcal{O}} \exists t.D'$, and thus $\sigma(C) \sqsubseteq_{\mathcal{O}}^s D$. Lemma 10 yields $\sigma(C) \sqsubseteq_{\mathcal{O}} D$.
- If there is a GCI $A_1 \sqcap \dots \sqcap A_k \sqsubseteq B$ in \mathcal{T} such that we have $B \sqsubseteq_{\mathcal{O}} D$ and $\tau([C \sqsubseteq A_1]^{i-1}) = \dots = \tau([C \sqsubseteq A_k]^{i-1}) = 1$, then $C = C$, $\text{Var}(D) = \text{Var}(A_1) = \dots = \text{Var}(A_k) = \perp$, and $i > i - 1$. By induction, we have $\sigma(C) \sqsubseteq_{\mathcal{O}} A_1, \dots, \sigma(C) \sqsubseteq_{\mathcal{O}} A_k$, and thus $\sigma(C) \sqsubseteq_{\mathcal{O}} A_1 \sqcap \dots \sqcap A_k \sqsubseteq_{\mathcal{O}} B \sqsubseteq_{\mathcal{O}} D$.

If D is neither ground nor a variable, we again consider C :

- If C is a variable, we again have $\sigma(C) \sqsubseteq \sigma(D)$ by the construction of σ .
- If C is not a variable, then one of the following cases must hold since τ satisfies the formulae in (II)3b):
 - If $C = D$, then obviously $C \sqsubseteq_{\mathcal{O}} D$ holds.
 - If $C = \exists r.C'$, $D = \exists s.D'$, $r \sqsubseteq_{\mathcal{O}} s$, and either $\tau([C' \sqsubseteq D']^{|\mathcal{T}|}) = 1$ or $\tau([C' \sqsubseteq \exists t.S']^{|\mathcal{T}|}) = 1$ for a transitive role name t with $r \sqsubseteq_{\mathcal{O}} t \sqsubseteq_{\mathcal{O}} s$, then $C >_{\sigma} C'$ since $\sigma(C) = \exists r.\sigma(C')$. Induction yields $\sigma(C') \sqsubseteq_{\mathcal{O}}^s \sigma(D)$, and thus $\sigma(C) \sqsubseteq_{\mathcal{O}} \sigma(D)$.
 - If there is an atom A in \mathcal{T} such that $\tau([C \sqsubseteq A]^i)$ and $\text{Dec}(A \sqsubseteq D)$ are both true, then $C = C$ and $\text{Var}(D) >_{\sigma} \perp = \text{Var}(A)$, and thus $\sigma(C) \sqsubseteq_{\mathcal{O}} A$ by induction. Furthermore, we have $A = \exists r.A'$, $D = \exists s.D'$, $r \sqsubseteq_{\mathcal{O}} s$, and either $\tau([A' \sqsubseteq D']^{|\mathcal{T}|}) = 1$ or $\tau([A' \sqsubseteq \exists t.D']^{|\mathcal{T}|}) = 1$ for a transitive role name t with $r \sqsubseteq_{\mathcal{O}} t \sqsubseteq_{\mathcal{O}} s$. Since $\sigma(C) \sqsubseteq_{\mathcal{O}} A = \exists r.A'$, we have $C > A'$, and thus we can apply induction to infer $A \sqsubseteq_{\mathcal{O}}^s \sigma(D)$, and thus $\sigma(C) \sqsubseteq_{\mathcal{O}} A \sqsubseteq_{\mathcal{O}} \sigma(D)$. \square

The next lemmata show that the same holds if the left-hand side of the subsumption is a conjunction $L \in \text{Left} \setminus \text{At}$. We first prove an auxiliary result.

Lemma 27. *If $\text{Dec}(C \sqsubseteq D)$ is evaluated to 1 under τ for $C \in \text{At}$, $D \in \text{At}_{\text{tr}}$, then $\sigma(C) \sqsubseteq_{\mathcal{O}} \sigma(D)$.*

Proof. We consider the cases in the definition of $\text{Dec}(C \sqsubseteq D)$.

- If $C = D$, then obviously $\sigma(C) \sqsubseteq_{\mathcal{O}} \sigma(D)$.
- If C and D are ground and $\tau([C \sqsubseteq D]^{|\mathcal{T}|}) = 1$, then $C \sqsubseteq_{\mathcal{O}} D$ must hold since otherwise τ would violate the clause $[C \sqsubseteq D]^{|\mathcal{T}|} \rightarrow$ in (II)1).

- If $C = \exists r.C'$, $D = \exists s.D'$, $r \trianglelefteq_{\mathcal{O}} s$ and either $\tau([C' \sqsubseteq D']^{|\mathcal{T}|}) = 1$ or $\tau([C' \sqsubseteq \exists t.D']^{|\mathcal{T}|}) = 1$ for a transitive role name t with $r \trianglelefteq_{\mathcal{O}} t \trianglelefteq_{\mathcal{O}} s$, then Lemma 26 yields $\sigma(C') \sqsubseteq_{\mathcal{O}} \sigma(D')$ or $\sigma(C') \sqsubseteq_{\mathcal{O}} \sigma(\exists t.D')$, respectively. Thus, we have $\sigma(C) \sqsubseteq_{\mathcal{O}}^s \sigma(D)$, which implies $\sigma(C) \sqsubseteq_{\mathcal{O}} \sigma(D)$.
- If C is a variable and $\tau([C \sqsubseteq D]^{|\mathcal{T}|}) = 1$, then by Lemma 26, we have $\sigma(C) \sqsubseteq_{\mathcal{O}} \sigma(D)$. \square

Lemma 28. *If $\tau([L \sqsubseteq D]^i) = 1$ for $L \in \text{Left} \setminus \text{At}$, $D \in \text{At}_{\text{tr}}$, and $i \in \{0, \dots, |\mathcal{T}|\}$, then $\sigma(L) \sqsubseteq_{\mathcal{O}} \sigma(D)$.*

Proof. We use well-founded induction on the lexicographic order on the pairs $(\text{Var}(D), i)$, where the components are compared as in Lemma 26.

If D is a variable and $\sigma(B)$ is a top-level atom of $\sigma(D)$, then by construction of σ we have $\tau([D \sqsubseteq B]^j) = 1$ for some $j \in \{0, \dots, |\mathcal{T}|\}$. By the formulae in (II)2), this implies $\tau([L \sqsubseteq B]^{\min\{|\mathcal{T}|, i+j\}}) = 1$. Since $\text{Var}(D) >_{\sigma} \text{Var}(B)$, by induction we know that $\sigma(L) \sqsubseteq_{\mathcal{O}} \sigma(B)$. Since this holds for all top-level atoms $\sigma(B)$ of $\sigma(D)$, we have $\sigma(L) \sqsubseteq_{\mathcal{O}} \sigma(D)$.

If D is a ground atom, then we know that τ satisfies the corresponding formulae in (II)3)a). If $\text{Dec}(C \sqsubseteq D)$ is true for some $C \in L$, then $\sigma(L) \sqsubseteq \sigma(C) \sqsubseteq_{\mathcal{O}} \sigma(D)$ by Lemma 27. Otherwise, there must be a GCI $A_1 \sqcap \dots \sqcap A_k \sqsubseteq B$ in \mathcal{T} with $B \sqsubseteq_{\mathcal{O}} D$ and $\tau([L \sqsubseteq A_1]^{i-1}) = \dots = \tau([L \sqsubseteq A_k]^{i-1}) = 1$. In this case, we have $\text{Var}(D) = \text{Var}(A_1) = \dots = \text{Var}(A_k) = \perp$ and $i > i - 1$, which implies that $\sigma(L) \sqsubseteq_{\mathcal{O}} A_1 \sqcap \dots \sqcap A_k \sqsubseteq_{\mathcal{O}} B \sqsubseteq_{\mathcal{O}} D$ by induction.

If D is neither ground nor a variable, then we consider the corresponding formulae in (II)3)b). If $\text{Dec}(C \sqsubseteq D)$ is true for $C \in L$, then we again have $\sigma(L) \sqsubseteq_{\mathcal{O}} \sigma(D)$ by Lemma 27. In the case that $\tau([L \sqsubseteq A]^i) = 1$ for some atom A of \mathcal{T} and $\text{Dec}(A \sqsubseteq D)$ is true, then $\text{Var}(D) >_{\sigma} \perp = \text{Var}(A)$, and thus $\sigma(L) \sqsubseteq_{\mathcal{O}} A \sqsubseteq_{\mathcal{O}} \sigma(D)$ by induction and Lemma 27. \square

Finally, since τ must satisfy the clauses in (I), by Lemmata 26 and 28 we know that σ solves Γ w.r.t. \mathcal{O} .

5.4 Completeness of the Reduction

Given a ground unifier γ of Γ w.r.t. \mathcal{O} , we can define a valuation τ that satisfies $C(\Gamma, \mathcal{O})$ as follows.

Let $L \in \text{Left}$ and $D \in \text{At}_{\text{tr}}$ and $i \in \{0, \dots, |\mathcal{T}|\}$. We set $\tau([L \sqsubseteq D]^i) := 1$ iff $\mathbf{s}(\gamma(L)) \stackrel{(i)}{\leftarrow}_{\mathcal{O}} \mathbf{s}(\gamma(D))$. According to Corollary 8, we thus have $\tau([L \sqsubseteq D]^i) = 0$ for all $i \in \{0, \dots, |\mathcal{T}|\}$ iff $\gamma(L) \not\sqsubseteq_{\mathcal{O}} \gamma(D)$. Otherwise, there is an $i \in \{0, \dots, |\mathcal{T}|\}$ such that $\tau([L \sqsubseteq D]^j) = 1$ for all $j \geq i$, and $\tau([L \sqsubseteq D]^j) = 0$ for all $j < i$.

To define the valuation of the remaining propositional variables $[X > Y]$ with $X, Y \in N_v$, we set $\tau([X > Y]) = 1$ iff $X >_\gamma Y$, where $>_\gamma$ is defined as before, i.e., $X >_\gamma Y$ iff $\gamma(X) \sqsubseteq_{\mathcal{O}} \exists w. \gamma(Y)$ for some $w \in N_R^+$.

Lemma 29. *Let $C \in \text{At}$, $D \in \text{At}_{\text{nv}}$, and E be a top-level atom of $\gamma(C)$ with $E \sqsubseteq_{\mathcal{O}}^s \gamma(D)$. Then $\text{Dec}(C \sqsubseteq D)$ is evaluated to 1 under τ .*

Proof. Consider the following cases:

- If $C = D$, then $\text{Dec}(C \sqsubseteq D) = \top$.
- If both C and D are ground, then $\text{Dec}(C \sqsubseteq D) = [C \sqsubseteq D]^{|\mathcal{T}|}$ and $\gamma(C) = C = E \sqsubseteq_{\mathcal{O}} D = \gamma(D)$. By Corollary 8, this implies $\gamma(C) \xleftarrow{(|\mathcal{T}|)}_{\mathcal{O}} \gamma(D)$, i.e., $\tau([C \sqsubseteq D]^{|\mathcal{T}|}) = 1$.
- If C is a concept name, then we again have $\gamma(C) \sqsubseteq_{\mathcal{O}} E \sqsubseteq_{\mathcal{O}} \gamma(D)$, and thus $\tau([C \sqsubseteq D]^{|\mathcal{T}|}) = 1$.
- If $C = \exists r.C'$, then $\gamma(C)$ is an atom, and thus $E = \gamma(C)$, $D = \exists s.D'$, $r \preceq_{\mathcal{O}} s$, and either $\gamma(C') \sqsubseteq_{\mathcal{O}} \gamma(D')$ or $\gamma(C') \sqsubseteq_{\mathcal{O}} \gamma(\exists t.D')$ for a transitive role name t with $r \preceq_{\mathcal{O}} t \preceq_{\mathcal{O}} s$. We obtain either $\tau([C' \sqsubseteq D']^{|\mathcal{T}|}) = 1$ or $\tau([C' \sqsubseteq \exists t.D']^{|\mathcal{T}|}) = 1$, i.e., $\text{Trans}(C \sqsubseteq D)$ is evaluated to 1 under τ . \square

Lemma 30. *The valuation τ satisfies $C(\Gamma, \mathcal{O})$.*

Proof. We consider the formulae introduced in Definition 24.

- (I) Since γ is a unifier of Γ w.r.t. \mathcal{O} , for every $L \sqsubseteq^? D$ in Γ we have $\gamma(L) \sqsubseteq_{\mathcal{O}} \gamma(D)$. By Corollary 8, this implies $\gamma(L) \xleftarrow{(|\mathcal{T}|)}_{\mathcal{O}} \gamma(D)$, and thus $\tau([L \sqsubseteq D]^{|\mathcal{T}|}) = 1$.
- (II) 1) If $C \sqsubseteq_{\mathcal{O}} D$ does not hold for two ground atoms $C \in \text{At}$, $D \in \text{At}_{\text{tr}}$, then $\gamma(C) \sqsubseteq_{\mathcal{O}} \gamma(D)$ does not hold, and thus $\tau([C \sqsubseteq D]^i) = 0$ for all $i \in \{0, \dots, |\mathcal{T}|\}$.
- 2) If $Y \in N_v$, $B \in \text{At}_{\text{nv}}$, $L \in \text{Left}$, and $i, j \in \{0, \dots, |\mathcal{T}|\}$ are such that $\tau([L \sqsubseteq Y]^i) = \tau([Y \sqsubseteq B]^j) = 1$, then $\gamma(L) \xleftarrow{(i)}_{\mathcal{O}} \gamma(Y) \xleftarrow{(j)}_{\mathcal{O}} \gamma(B)$, and thus $\gamma(L) \xleftarrow{(i+j)}_{\mathcal{O}} \gamma(B)$. By Lemma 7, there must be a derivation of $\gamma(L)$ from $\gamma(B)$ that uses at most $\min\{|\mathcal{T}|, i+j\}$ root steps, and thus $\tau([L \sqsubseteq B]^{\min\{|\mathcal{T}|, i+j\}}) = 1$.
- 3) Let $L \in \text{Left} \setminus N_v$, $D \in \text{At}_{\text{tr}}$, and $i \in \{0, \dots, |\mathcal{T}|\}$ satisfy $\tau([L \sqsubseteq D]^i) = 1$, i.e., $\gamma(L) \xleftarrow{(i)}_{\mathcal{O}} \gamma(D)$.
- a) If D is a ground atom and L is not a ground atom, then by Lemma 11 we have one of the following cases:

- If there is $C \in L$ such that $E \sqsubseteq_{\mathcal{O}}^s D$ for some top-level atom E of $\gamma(C)$, then by Lemma 29 $\text{Dec}(C \sqsubseteq D)$ is evaluated to 1.
- Otherwise, there must be a GCI $A_1 \sqcap \dots \sqcap A_k \sqsubseteq B$ in \mathcal{T} with $\gamma(L) \stackrel{(i-1)}{\leftarrow}_{\mathcal{O}} A_1, \dots, \gamma(L) \stackrel{(i-1)}{\leftarrow}_{\mathcal{O}} A_k$, and $B \sqsubseteq_{\mathcal{O}}^s D$. Note that this is only possible with $i > 0$. We then have $\tau([L \sqsubseteq A_1]^{i-1}) = \dots = \tau([L \sqsubseteq A_k]^{i-1}) = 1$ and $B \sqsubseteq_{\mathcal{O}} D$.

b) If D is a non-variable, non-ground atom, then by Lemma 11 we have one of the following cases:

- If there is $C \in L$ such that $E \sqsubseteq_{\mathcal{O}}^s \gamma(D)$ for some top-level atom E of $\gamma(C)$, then by Lemma 29 $\text{Dec}(C \sqsubseteq D)$ is evaluated to 1.
- If there is a GCI $A_1 \sqcap \dots \sqcap A_k \sqsubseteq B \in \mathcal{T}$ with $\gamma(L) \stackrel{(i)}{\leftarrow}_{\mathcal{O}} B$ and $B \sqsubseteq_{\mathcal{O}}^s \gamma(D)$, then $\tau([L \sqsubseteq B]^i) = 1$ and $\text{Dec}(B \sqsubseteq D)$ is evaluated to 1.

(III) 1) Assume that $\tau([X > X]) = 1$ for some variable $X \in N_v$. By the definition of $>_{\gamma}$, this implies that $\gamma(X) \sqsubseteq_{\mathcal{O}} \exists w.\gamma(X)$ for some $w \in N_R^+$. This contradicts the assumption that \mathcal{O} is cycle-restricted.

Moreover, if $\tau([X > Y]) = \tau([Y > Z]) = 1$, then $\gamma(X) \sqsubseteq_{\mathcal{O}} \exists w w'.\gamma(Z)$ with $w, w' \in N_R^+$, and thus $\tau([X > Z]) = 1$.

2) If $\tau([X \sqsubseteq \exists r.Y]^i) = 1$, then $\gamma(X) \stackrel{(i)}{\leftarrow}_{\mathcal{O}} \exists r.\gamma(Y)$, which implies $\gamma(X) \sqsubseteq_{\mathcal{O}} \exists r.\gamma(Y)$. By the definition of $>_{\gamma}$, we thus have $\tau([X > Y]) = 1$. \square

This completes the proof of correctness of the presented reduction.

Theorem 31. *Unification w.r.t. cycle-restricted \mathcal{ELH}_{R^+} -ontologies is an NP-complete problem.*

Proof. NP-hardness follows from NP-hardness of unification in \mathcal{EL} w.r.t. the empty ontology [5]. The other direction is provided by the presented reduction to the NP-complete SAT problem. \square

This also shows locality of unification w.r.t. cycle-restricted \mathcal{ELH}_{R^+} -ontologies, i.e., in this setting a unification problem has a unifier iff it has a local unifier.

Lemma 32. *If a flat unification problem Γ has a unifier w.r.t. a flat, cycle-restricted \mathcal{ELH}_{R^+} -ontology \mathcal{O} , then it has a local unifier w.r.t. \mathcal{O} .*

Proof. If Γ has a unifier w.r.t. \mathcal{O} , then $C(\Gamma, \mathcal{O})$ is satisfiable by Lemma 30. Thus, Section 5.3 shows that there is a local unifier of Γ w.r.t. \mathcal{O} . \square

6 Conclusions

We have shown that unification w.r.t. cycle-restricted \mathcal{ELH}_{R^+} -ontologies can be reduced to propositional satisfiability. This improves on the results in [2] in two respects. First, it allows us to deal also with ontologies that contain transitivity and role hierarchy axioms, which are important for medical ontologies. Second, the SAT reduction can easily be implemented and enables us to make use of highly optimized SAT solvers, whereas the goal-oriented algorithm in [1], while having the potential of becoming quite efficient, requires a high amount of additional optimization work. The main topic for future research is to investigate whether we can get rid of cycle-restrictedness.

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