

# Query-Based Entailment and Inseparability for $\mathcal{ALC}$ Ontologies

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## Abstract

We investigate the problem whether two  $\mathcal{ALC}$  knowledge bases are indistinguishable by queries over a given vocabulary. We give model-theoretic criteria and prove that this problem is undecidable for conjunctive queries (CQs) but decidable in 2EXPTIME for unions of rooted CQs. We also consider the problem whether two  $\mathcal{ALC}$  TBoxes give the same answers to any query in a given vocabulary over all ABoxes, and show that for CQs this problem is undecidable, too, but becomes decidable and 2EXPTIME-complete in *Horn- $\mathcal{ALC}$* , and even EXPTIME-complete in *Horn- $\mathcal{ALC}$*  when restricted to (unions of) rooted CQs.

## 1 Introduction

In recent years, data access using description logic (DL) TBoxes has become one of the most important applications of DLs [Poggi *et al.*, 2008; Bienvenu and Ortiz, 2015], where the underlying idea is to use a TBox to specify semantics and background knowledge for the data (stored in an ABox), and thereby derive more complete query answers. A major research effort has led to the development of efficient algorithms and tools for a number of DLs ranging from DL-Lite [Calvanese *et al.*, 2007; Rodriguez-Muro *et al.*, 2013] via more expressive Horn DLs such as Horn- $\mathcal{ALC}$  [Eiter *et al.*, 2012; Trivela *et al.*, 2015] to DLs with all Boolean constructors such as  $\mathcal{ALC}$  [Kollia and Glimm, 2013; Zhou *et al.*, 2015].

While query answering with DLs is now well-developed, this is much less the case for reasoning services that support ontology engineering and target query answering as an application. In ontology versioning, for example, one would like to know whether two versions of an ontology give the same answers to all queries formulated over a given vocabulary of interest, which means that the newer version can safely replace the older one [Konev *et al.*, 2012]. Similarly, if one wants to know whether an ontology can be safely replaced by a smaller subset (module), it is the answers to all queries that should be preserved [Kontchakov *et al.*, 2010]. In this context, the fundamental relationship between ontologies is thus not whether they are logically equivalent (have the same models), but whether they give the same answers to any relevant query.

The resulting entailment problem can be formalized in two ways, with different applications. First, given a class  $\mathcal{Q}$  of queries, knowledge bases (KBs)  $\mathcal{K}_1$  and  $\mathcal{K}_2$ , and a signature  $\Sigma$  of relevant concept and role names, we say that  $\mathcal{K}_1$   $\Sigma$ - $\mathcal{Q}$ -entails  $\mathcal{K}_2$  if the answers to any  $\Sigma$ -query in  $\mathcal{Q}$  over  $\mathcal{K}_2$  are contained in the answers to the same query over  $\mathcal{K}_1$ . Further,  $\mathcal{K}_1$  and  $\mathcal{K}_2$  are  $\Sigma$ - $\mathcal{Q}$ -inseparable if they  $\Sigma$ - $\mathcal{Q}$ -entail each other. Note that a KB includes an ABox, and thus this notion of entailment is appropriate if the data is known and does not change frequently. Applications include data-oriented KB versioning and KB module extraction, KB forgetting [Wang *et al.*, 2014], and knowledge exchange [Arenas *et al.*, 2013].

If the data is not known or changes frequently, it is not KBs that should be compared, but TBoxes. Given a pair  $\Theta = (\Sigma_1, \Sigma_2)$  that specifies a relevant signature  $\Sigma_1$  for ABoxes and  $\Sigma_2$  for queries, we say that a TBox  $\mathcal{T}_1$   $\Theta$ - $\mathcal{Q}$ -entails a TBox  $\mathcal{T}_2$  if, for every  $\Sigma_1$ -ABox  $\mathcal{A}$ , the KB  $(\mathcal{T}_1, \mathcal{A})$   $\Sigma_2$ - $\mathcal{Q}$ -entails  $(\mathcal{T}_2, \mathcal{A})$ .  $\mathcal{T}_1$  and  $\mathcal{T}_2$  are  $\Theta$ - $\mathcal{Q}$ -inseparable if they  $\Theta$ - $\mathcal{Q}$ -entail each other. Applications include data-oriented TBox versioning, TBox modularization and TBox forgetting [Kontchakov *et al.*, 2010].

In this paper, we concentrate on the most important choices for  $\mathcal{Q}$ , conjunctive queries (CQs) and unions thereof (UCQs); we also consider the practically relevant classes of rooted CQs (rCQs) and UCQs (rUCQs), in which every variable is connected to an answer variable. So far, CQ-entailment has been studied for Horn DL KBs [Botoeva *et al.*, 2014],  $\mathcal{EL}$  TBoxes [Lutz and Wolter, 2010; Konev *et al.*, 2012], DL-Lite TBoxes [Kontchakov *et al.*, 2009], and also for OBDA specifications, that is, DL-Lite TBoxes with mappings [Bienvenu and Rosati, 2015]. No results are available for non-Horn DLs (neither in the KB nor in the TBox case) and for expressive Horn DLs in the TBox case. In particular, query entailment in non-Horn DLs has had the reputation of being a technically challenging problem.

This paper makes a first breakthrough into understanding query entailment and inseparability in these cases, with the main results summarized in Figures 1 and 2 (those marked with  $(\star)$  are from [Botoeva *et al.*, 2014]). Three of them came as a real surprise to us. First, it turned out that CQ- and rCQ-entailment between  $\mathcal{ALC}$  KBs is undecidable, even when the first KB is formulated in *Horn- $\mathcal{ALC}$*  (in fact,  $\mathcal{EL}$ ) and without any signature restriction. This should be contrasted with the decidability of subsumption-based entailment between  $\mathcal{ALC}$

Queries	$\mathcal{ALC}$	$\text{Horn-}\mathcal{ALC}$ to $\mathcal{ALC}$	$\mathcal{ALC}$ to $\text{Horn-}\mathcal{ALC}$	$\text{Horn-}\mathcal{ALC}$
CQ	undecidable		?	=EXPTIME <sup>(*)</sup>
UCQ	?			
rCQ	undecidable		$\leq 2\text{EXPTIME}$	=EXPTIME <sup>(*)</sup>
rUCQ	$\leq 2\text{EXPTIME}$			

Figure 1: KB query entailment.

TBoxes [Ghilardi *et al.*, 2006] and of CQ-entailment between  $\text{Horn-}\mathcal{ALC}$  KBs [Botoeva *et al.*, 2014]. The second surprising result is that entailment between  $\mathcal{ALC}$  KBs becomes decidable when CQs are replaced with rUCQs. For  $\mathcal{ALC}$  TBoxes, CQ- and rCQ-entailment are undecidable as well. We obtain decidability for  $\text{Horn-}\mathcal{ALC}$  TBoxes (where CQ- und UCQ-entailments coincide) using the fact that non-entailment is always witnessed by tree-shaped ABoxes. As another surprise, CQ-entailment of  $\text{Horn-}\mathcal{ALC}$  TBoxes is 2EXPTIME-complete while rCQ-entailment is only EXPTIME-complete. This should be contrasted with the  $\mathcal{EL}$  case, where both problems are EXPTIME-complete [Lutz and Wolter, 2010]. All upper bounds and most lower bounds hold also for inseparability in place of entailment. A model-theoretic foundation for these results is a characterization of query entailment between KBs and TBoxes in terms of (partial) homomorphisms, which, in particular, enables the use of tree automata techniques to establish the upper bounds in Figs. 1 and 2. Omitted proofs are available in the full version [Botoeva *et al.*, 2016].

## 2 Preliminaries

Fix lists of *individual names*  $a_i$ , *concept names*  $A_i$ , and *role names*  $R_i$ , for  $i < \omega$ .  $\mathcal{ALC}$ -concepts,  $C$ , are defined by the grammar

$$C ::= A_i \mid \top \mid \neg C \mid C_1 \sqcap C_2 \mid \exists R_i.C.$$

We use  $\perp$ ,  $C_1 \sqcup C_2$  and  $\forall R.C$  as abbreviations for  $\neg\top$ ,  $\neg(\neg C_1 \sqcap \neg C_2)$  and  $\neg\exists R.\neg C$ , respectively. A *concept inclusion* (CI) takes the form  $C \sqsubseteq D$ , where  $C$  and  $D$  are concepts. An  $\mathcal{ALC}$  TBox is a finite set of CIs. In a  $\text{Horn-}\mathcal{ALC}$  TBox, no concept of the form  $\neg C$  occurs negatively and no  $\exists R.\neg C$  occurs positively [Hustadt *et al.*, 2005; Kazakov, 2009]. An  $\mathcal{EL}$  TBox does not contain  $\neg$  at all. An ABox,  $\mathcal{A}$ , is a finite set of *assertions* of the form  $A_k(a_i)$  or  $R_k(a_i, a_j)$ ;  $\text{ind}(\mathcal{A})$  is the set of individual names in  $\mathcal{A}$ . Taken together,  $\mathcal{T}$  and  $\mathcal{A}$  form a *knowledge base* (KB)  $\mathcal{K} = (\mathcal{T}, \mathcal{A})$ ; we set  $\text{ind}(\mathcal{K}) = \text{ind}(\mathcal{A})$ .

The semantics is defined as usual based on interpretations  $\mathcal{I} = (\Delta^{\mathcal{I}}, \cdot^{\mathcal{I}})$  that comply with the *standard name assumption* in the sense that  $a_i^{\mathcal{I}} = a_i$  [Baader *et al.*, 2003]. We write  $\mathcal{I} \models \alpha$  if an inclusion or assertion  $\alpha$  is true in  $\mathcal{I}$ . If  $\mathcal{I} \models \alpha$ , for all  $\alpha \in \mathcal{T} \cup \mathcal{A}$ , then we call  $\mathcal{I}$  a *model* of  $\mathcal{K}$  and write  $\mathcal{I} \models \mathcal{K}$ .  $\mathcal{K}$  is *consistent* if it has a model; we then also say that  $\mathcal{A}$  is *consistent with*  $\mathcal{T}$ .  $\mathcal{K} \models \alpha$  means that  $\mathcal{I} \models \alpha$  for all  $\mathcal{I} \models \mathcal{K}$ .

A *conjunctive query* (CQ)  $q(x)$  is a formula  $\exists \mathbf{y} \varphi(x, \mathbf{y})$ , where  $\varphi$  is a conjunction of atoms of the form  $A_k(z_1)$  or  $R_k(z_1, z_2)$  with  $z_i$  in  $\mathbf{x}, \mathbf{y}$ ; the variables in  $\mathbf{x}$  are the *answer variables* of  $q(x)$ . We call  $q$  *rooted* (rCQ) if every  $y \in \mathbf{y}$  is connected to some  $x \in \mathbf{x}$  by a path in the graph whose

Queries	$\mathcal{ALC}$	$\text{Horn-}\mathcal{ALC}$ to $\mathcal{ALC}$	$\mathcal{ALC}$ to $\text{Horn-}\mathcal{ALC}$	$\text{Horn-}\mathcal{ALC}$
CQ	undecidable		?	=2EXPTIME
UCQ	?			
rCQ	undecidable		=EXPTIME	=EXPTIME
rUCQ	?			

Figure 2: TBox query entailment.

nodes are the variables in  $q$  and edges are the pairs  $\{u, v\}$  with  $R(u, v) \in q$ , for some  $R$ . A *union of CQs* (UCQ) is a disjunction  $q(x) = \bigvee_i q_i(x)$  of CQs  $q_i(x)$  with the same *answer variables*  $\mathbf{x}$ ; it is *rooted* (rUCQ) if all  $q_i$  are rooted.

A tuple  $\mathbf{a}$  in  $\text{ind}(\mathcal{K})$  is a *certain answer to a UCQ*  $q(x)$  over  $\mathcal{K} = (\mathcal{T}, \mathcal{A})$  if  $\mathcal{I} \models q(\mathbf{a})$  for all  $\mathcal{I} \models \mathcal{K}$ ; in this case we write  $\mathcal{K} \models q(\mathbf{a})$ . If  $\mathbf{x} = \emptyset$ , the answer to  $q$  is ‘yes’ if  $\mathcal{K} \models q$  and ‘no’ otherwise. The problem of checking whether a tuple is a certain answer to a given (U)CQ over a given  $\mathcal{ALC}$  KB is known to be EXPTIME-complete for combined complexity [Lutz, 2008]. The EXPTIME lower bound actually holds for  $\text{Horn-}\mathcal{ALC}$  [Krötzsch *et al.*, 2013].

A set  $\mathcal{M}$  of models of a KB  $\mathcal{K}$  is called *complete for*  $\mathcal{K}$  if, for every UCQ  $q(x)$ , we have  $\mathcal{K} \models q(\mathbf{a})$  iff  $\mathcal{I} \models q(\mathbf{a})$  for all  $\mathcal{I} \in \mathcal{M}$ . We call an interpretation  $\mathcal{I}$  a *ditree interpretation* if the directed graph  $G_{\mathcal{I}}$  with nodes  $d \in \Delta^{\mathcal{I}}$  and edges  $(d, e) \in R^{\mathcal{I}}$ , for some  $R$ , is a tree and  $R^{\mathcal{I}} \cap S^{\mathcal{I}} = \emptyset$ , for any distinct roles  $R$  and  $S$ .  $\mathcal{I}$  has *outdegree*  $n$  if  $G_{\mathcal{I}}$  has outdegree  $n$ . A model  $\mathcal{I}$  of a KB  $\mathcal{K} = (\mathcal{T}, \mathcal{A})$  is *forest-shaped* if  $\mathcal{I}$  is the disjoint union of ditree interpretations  $\mathcal{I}_a$  with root  $a$ , for  $a \in \text{ind}(\mathcal{A})$ , extended with all  $R(a, b) \in \mathcal{A}$ . The *outdegree* of  $\mathcal{I}$  is the maximum outdegree of the  $\mathcal{I}_a$ . It is well known that the class  $\mathcal{M}_{\mathcal{K}}^{\text{fo}}$  of all forest-shaped models of an  $\mathcal{ALC}$  KB  $\mathcal{K}$  of outdegree bounded by  $|\mathcal{T}|$  is complete for  $\mathcal{K}$  [Lutz, 2008]. If  $\mathcal{K}$  is a  $\text{Horn-}\mathcal{ALC}$  KB, then a single member  $\mathcal{I}_{\mathcal{K}}$  of  $\mathcal{M}_{\mathcal{K}}^{\text{fo}}$  is complete for  $\mathcal{K}$ .  $\mathcal{I}_{\mathcal{K}}$  is constructed using the standard chase procedure and called the *canonical model* of  $\mathcal{K}$ .

A *signature*,  $\Sigma$ , is a set of concept and role names. By a  $\Sigma$ -concept,  $\Sigma$ -CQ, etc. we understand any concept, CQ, etc. constructed using the names from  $\Sigma$ . We say that  $\Sigma$  is *full* if it contains all concept and role names. A model  $\mathcal{I}$  of a KB  $\mathcal{K}$  is  $\Sigma$ -connected if, for any  $u \in \Delta^{\mathcal{I}} \setminus \text{ind}(\mathcal{K})$ , there is a path  $R_1^{\mathcal{I}}(a, u_1), \dots, R_n^{\mathcal{I}}(u_n, u)$  with  $a \in \text{ind}(\mathcal{K})$  and the  $R_i$  in  $\Sigma$ .

**Definition 1.** Let  $\mathcal{K}_1$  and  $\mathcal{K}_2$  be consistent KBs,  $\Sigma$  a signature, and  $\mathcal{Q}$  one of CQ, rCQ, UCQ or rUCQ. We say that  $\mathcal{K}_1$   $\Sigma$ - $\mathcal{Q}$ -entails  $\mathcal{K}_2$  if  $\mathcal{K}_2 \models q(\mathbf{a})$  implies  $\mathbf{a} \subseteq \text{ind}(\mathcal{K}_1)$  and  $\mathcal{K}_1 \models q(\mathbf{a})$ , for all  $\Sigma$ - $\mathcal{Q}$   $q(x)$  and all tuples  $\mathbf{a}$  in  $\text{ind}(\mathcal{K}_2)$ .  $\mathcal{K}_1$  and  $\mathcal{K}_2$  are  $\Sigma$ - $\mathcal{Q}$  inseparable if they  $\Sigma$ - $\mathcal{Q}$  entail each other.

As larger classes of queries separate more KBs,  $\Sigma$ -UCQ inseparability implies all other inseparabilities. The following example shows that, in general, no other implications between the different notions of inseparability hold for  $\mathcal{ALC}$ .

**Example 2.** Suppose  $\mathcal{T}_0 = \emptyset$ ,  $\mathcal{T}'_0 = \{E \sqsubseteq A \sqcup B\}$  and  $\Sigma_0 = \{A, B, E\}$ . Let  $\mathcal{A}_0 = \{E(a)\}$ ,  $\mathcal{K}_0 = (\mathcal{T}_0, \mathcal{A}_0)$ , and  $\mathcal{K}'_0 = (\mathcal{T}'_0, \mathcal{A}_0)$ . Then  $\mathcal{K}_0$  and  $\mathcal{K}'_0$  are  $\Sigma_0$ -CQ inseparable but not  $\Sigma_0$ -rUCQ inseparable. In fact,  $\mathcal{K}'_0 \models q(\mathbf{a})$  and  $\mathcal{K}_0 \not\models q(\mathbf{a})$  for  $q(x) = A(x) \vee B(x)$ .

Now, let  $\Sigma_1 = \{E, B\}$ ,  $\mathcal{T}_1 = \emptyset$ , and  $\mathcal{T}'_1 = \{E \sqsubseteq \exists R.B\}$ . Let  $\mathcal{A}_1 = \{E(a)\}$ ,  $\mathcal{K}_1 = (\mathcal{T}_1, \mathcal{A}_1)$ , and  $\mathcal{K}'_1 = (\mathcal{T}'_1, \mathcal{A}_1)$ .





## 5 rUCQ-Entailment for $\mathcal{ALC}$ -KBs

Theorem 7 might seem to suggest that any reasonable notion of query inseparability is undecidable for  $\mathcal{ALC}$  KBs. Interestingly, this is not the case: we show now that rUCQ-entailment is decidable. We first strengthen the characterization of Theorem 6 (2), and then develop a decision procedure based on tree automata. The first step replaces con- $n\Sigma$ -homomorphic embeddability with con- $\Sigma$ -homomorphic embeddability, where  $\mathcal{I}_2$  is *con- $\Sigma$ -homomorphically embeddable into  $\mathcal{I}_1$*  if the maximal  $\Sigma$ -connected subinterpretation of  $\mathcal{I}_2$  is  $\Sigma$ -homomorphically embeddable into  $\mathcal{I}_1$ .

**Theorem 10.** *Let  $\mathcal{K}_1$  and  $\mathcal{K}_2$  be  $\mathcal{ALC}$  KBs,  $\Sigma$  a signature, and let  $\mathcal{M}_1$  be complete for  $\mathcal{K}_1$ . Then  $\mathcal{K}_1 \Sigma$ -rUCQ entails  $\mathcal{K}_2$  iff for any  $\mathcal{I}_1 \in \mathcal{M}_1$ , there exists  $\mathcal{I}_2 \models \mathcal{K}_2$  such that  $\mathcal{I}_2$  is con- $\Sigma$ -homomorphically embeddable into  $\mathcal{I}_1$ .*

*Proof.* In view of Theorem 6 (2), it suffices to prove ( $\Rightarrow$ ). Suppose  $\mathcal{I}_1 \in \mathcal{M}_1$ . By Theorem 6 (2), for every  $n \geq 0$ , we have  $\mathcal{J} \in M_{\mathcal{K}_2}^{fo}$  and a  $\Sigma$ -homomorphism  $h_n: \mathcal{J}_{\leq n} \rightarrow \mathcal{I}_1$ , where  $\mathcal{J}_{\leq n}$  is the subinterpretation of  $\mathcal{J}$  whose elements are connected to ABox individuals by  $\Sigma$ -paths of length  $\leq n$ . Clearly, for any  $n \geq 0$ , there are only finitely many non-isomorphic pairs  $(\mathcal{J}_{\leq n}, h_n)$ . It can be shown that, thus, one can construct the required  $\mathcal{I}_2 \in M_{\mathcal{K}_2}^{fo}$  and con- $\Sigma$ -homomorphism  $h$  as the limits of suitable chains  $\mathcal{J}_{\leq 0} \subseteq \mathcal{J}_{\leq 1} \subseteq \dots$  and  $h_0 \subseteq h_1 \subseteq \dots$ , respectively.  $\square$

For the second step, let  $\mathcal{K}_1, \mathcal{K}_2$  be  $\mathcal{ALC}$ -KBs and  $\Sigma$  a signature. We use two-way alternating automata on infinite trees (2ATAs) with a trivial acceptance condition (every run is accepting) and employ Theorem 10 for the class  $M_{\mathcal{K}_1}^{fo}$ , encoding forest-shaped interpretations as labeled trees to make them accessible to 2ATAs. A *tree* is a non-empty (possibly infinite) set  $T \subseteq \mathbb{N}^*$  closed under prefixes with root  $\varepsilon$ . We say that  $T$  is *m-ary* if, for every  $x \in T$ , the set  $\{i \mid x \cdot i \in T\}$  is of cardinality  $m$ . Let  $\Gamma$  be an alphabet with symbols from the set

$$\{\text{root}, \text{empty}\} \cup (\text{ind}(\mathcal{K}_1) \times 2^{\text{CN}(\mathcal{T}_1)}) \cup (\text{RN}(\mathcal{T}_1) \times 2^{\text{CN}(\mathcal{T}_1)}),$$

where  $\text{CN}(\mathcal{T}_i)$  (resp.  $\text{RN}(\mathcal{T}_i)$ ) denotes the set of concept (resp. role) names in  $\mathcal{T}_i$ . A  $\Gamma$ -labeled tree is a pair  $(T, L)$  with  $T$  a tree and  $L: T \rightarrow \Gamma$  a node labeling function. We represent forest-shaped models of  $\mathcal{T}_1$  as  $m$ -ary  $\Gamma$ -labeled trees, with  $m = \max(|\mathcal{T}_1|, |\text{ind}(\mathcal{K}_1)|)$ . The root node labeled with *root* is not used in the representation. Each ABox individual is represented by a successor of the root labeled with a symbol from  $\text{ind}(\mathcal{K}_1) \times 2^{\text{CN}(\mathcal{T}_1)}$ ; non-ABox elements are represented by nodes deeper in the tree labeled with a symbol from  $\text{RN}(\mathcal{T}_1) \times 2^{\text{CN}(\mathcal{T}_1)}$ . The label *empty* is used for padding to make sure that every tree node has exactly  $m$  successors.

Now we construct three 2ATAs  $\mathfrak{A}_i$ , for  $i = 0, 1, 2$ .  $\mathfrak{A}_0$  ensures that the tree is labeled in a meaningful way, e.g. that the *root* label only occurs at the root node;  $\mathfrak{A}_1$  accepts  $\Gamma$ -labeled trees that represent a model of  $\mathcal{K}_1$ , and  $\mathfrak{A}_2$  accepts  $\Gamma$ -labeled trees  $(T, L)$  which represent an interpretation  $\mathcal{I}_{(T,L)}$  such that some model of  $\mathcal{K}_2$  is con- $\Sigma$ -homomorphically embeddable into  $\mathcal{I}_{(T,L)}$ . The most interesting automaton is  $\mathfrak{A}_2$ , which guesses a model of  $\mathcal{K}_2$  along with a homomorphism to  $\mathcal{I}_{(T,L)}$ ;

in fact, both can be read off from a successful run of the automaton. The number of states of the  $\mathfrak{A}_i$  is exponential in  $|\mathcal{K}_1 \cup \mathcal{K}_2|$ . It then remains to combine these automata into a single 2ATA  $\mathfrak{A}$  such that  $\mathcal{L}(\mathfrak{A}) = \mathcal{L}(\mathfrak{A}_0) \cap \mathcal{L}(\mathfrak{A}_1) \cap \overline{\mathcal{L}(\mathfrak{A}_2)}$ , which is possible with only polynomial blowup, and to test (in time exponential in the number of states) whether  $\mathcal{L}(\mathfrak{A}) = \emptyset$ .

**Theorem 11.** *It is in 2EXPTIME to decide whether an  $\mathcal{ALC}$  KB  $\mathcal{K}_1 \Sigma$ -rUCQ entails an  $\mathcal{ALC}$  KB  $\mathcal{K}_2$ .*

The best known lower bound is EXPTIME, which is easy to establish by reduction from satisfiability.

## 6 (r)CQ-Entailment for (Horn-) $\mathcal{ALC}$ -TBoxes

We show that CQ- and rCQ-entailment between  $\mathcal{ALC}$  TBoxes becomes decidable when the second TBox is given in Horn- $\mathcal{ALC}$ . In this case, entailments for CQs and UCQs and, respectively, rCQs and rUCQs coincide. We start with rCQs.

Our first observation is that if a  $\Sigma_1$ -ABox is a witness for non- $\Theta$ -rCQ entailment, then one can find a witness  $\Sigma_1$ -ABox that is tree-shaped and of bounded outdegree. Here, an ABox  $\mathcal{A}$  is *tree-shaped* if the graph with nodes  $\text{ind}(\mathcal{A})$  and edges  $\{a, b\}$  for each  $R(a, b) \in \mathcal{A}$  is a tree, and  $R(a, b) \in \mathcal{A}$  implies  $S(a, b) \notin \mathcal{A}$  for all  $S \neq R$  and  $S(b, a) \notin \mathcal{A}$  for all  $S$ .

**Theorem 12.** *Let  $\mathcal{T}_1$  be an  $\mathcal{ALC}$  TBox,  $\mathcal{T}_2$  a Horn- $\mathcal{ALC}$  TBox, and  $\Theta = (\Sigma_1, \Sigma_2)$ . Then  $\mathcal{T}_1 \Theta$ -rCQ-entails  $\mathcal{T}_2$  iff, for all tree-shaped  $\Sigma_1$ -ABoxes  $\mathcal{A}$  of outdegree bounded by  $|\mathcal{T}_2|$  and consistent with  $\mathcal{T}_1$  and  $\mathcal{T}_2$ ,  $\mathcal{I}_{\mathcal{T}_2, \mathcal{A}}$  is con- $\Sigma_2$ -homomorphically embeddable into any model  $\mathcal{I}_1$  of  $(\mathcal{T}_1, \mathcal{A})$ .*

*Proof.* It is known that Horn- $\mathcal{ALC}$  is unravelling tolerant, that is,  $(\mathcal{T}, \mathcal{A}) \models C(a)$  for a Horn- $\mathcal{ALC}$  TBox  $\mathcal{T}$  and  $\mathcal{EL}$ -concept  $C$  iff  $(\mathcal{T}, \mathcal{A}') \models C(a)$  for a finite sub-ABox  $\mathcal{A}'$  of the tree-unravelling of  $\mathcal{A}$  at  $a$  [Lutz and Wolter, 2012]. Thus, any witness ABox for non-entailment w.r.t.  $\mathcal{EL}$ -instance queries can be transformed into a tree-shaped witness ABox. The result follows by observing that if  $\mathcal{T}_1$  does not  $\Theta$ -rCQ-entail  $\mathcal{T}_2$ , then this is witnessed by an  $\mathcal{EL}$ -instance query and by applying Theorem 10 to the KBs. The bound on the outdegree is obtained by a careful analysis of derivations.  $\square$

For the automaton construction, let  $\mathcal{T}_1$  be an  $\mathcal{ALC}$  TBox,  $\mathcal{T}_2$  a Horn- $\mathcal{ALC}$  TBox, and  $\Theta = (\Sigma_1, \Sigma_2)$  a pair of signatures. Though Theorem 12 provides a natural characterization that is similar in spirit to Theorem 10, we first need a further analysis of con- $\Sigma_2$ -homomorphic embeddability in terms of simulations whose advantage is that they are more compositional (they can be partial and are closed under union).

Let  $\mathcal{I}_1, \mathcal{I}_2$  be interpretations and  $\Sigma$  a signature. A relation  $\mathcal{S} \subseteq \Delta^{\mathcal{I}_1} \times \Delta^{\mathcal{I}_2}$  is a  $\Sigma$ -simulation from  $\mathcal{I}_1$  to  $\mathcal{I}_2$  if (i)  $d \in A^{\mathcal{I}_1}$  and  $(d, d') \in \mathcal{S}$  imply  $d' \in A^{\mathcal{I}_2}$  for all  $\Sigma$ -concept names  $A$ , and (ii) if  $(d, e) \in R^{\mathcal{I}_1}$  and  $(d, d') \in \mathcal{S}$  then there is a  $(d', e') \in R^{\mathcal{I}_2}$  with  $(e, e') \in \mathcal{S}$  for all  $\Sigma$ -role names  $R$ . Let  $d_i \in \Delta^{\mathcal{I}_i}$ ,  $i \in \{1, 2\}$ .  $(\mathcal{I}_1, d_1)$  is  $\Sigma$ -simulated by  $(\mathcal{I}_2, d_2)$ , in symbols  $(\mathcal{I}_1, d_1) \leq_{\Sigma} (\mathcal{I}_2, d_2)$ , if there exists a  $\Sigma$ -simulation  $\mathcal{S}$  with  $(d_1, d_2) \in \mathcal{S}$ .

**Lemma 13.** *Let  $\mathcal{A}$  be a  $\Sigma_1$ -ABox and  $\mathcal{I}_1$  a model of  $(\mathcal{T}_1, \mathcal{A})$ . Then  $\mathcal{I}_{\mathcal{T}_2, \mathcal{A}}$  is not con- $\Sigma_2$ -homomorphically embeddable into  $\mathcal{I}_1$  iff there is a  $a \in \text{ind}(\mathcal{A})$  such that one of the following holds:*

- (1) *there is a  $\Sigma_2$ -concept name  $A$  with  $a \in A^{\mathcal{I}_{\mathcal{T}_2, \mathcal{A}}} \setminus A^{\mathcal{I}_1}$ ;*
- (2) *there is an  $R$ -successor  $d$  of  $a$  in  $\mathcal{I}_{\mathcal{T}_2, \mathcal{A}}$ , for some  $\Sigma_2$ -role name  $R$ , such that  $d \notin \text{ind}(\mathcal{A})$  and, for all  $R$ -successors  $e$  of  $a$  in  $\mathcal{I}_1$ , we have  $(\mathcal{I}_{\mathcal{T}_2, \mathcal{A}}, d) \not\leq_{\Sigma_2} (\mathcal{I}_1, e)$ .*

We use a mix of two-way alternating Büchi automata on finite trees (2ABTAs) and non-deterministic top-down automata on finite trees (NTAs). A finite tree  $T$  is  $m$ -ary if, for every  $x \in T$ , the set  $\{i \mid x \cdot i \in T\}$  is of cardinality zero or exactly  $m$ . We use labeled trees to represent a tree-shaped ABox  $\mathcal{A}$  and a model  $\mathcal{I}_1$  such that, for some  $a \in \text{ind}(\mathcal{A})$ , conditions (1) and (2) from Lemma 13 are satisfied, and thus  $\mathcal{I}_{\mathcal{T}_2, \mathcal{A}}$  is not con- $\Sigma_2$ -homomorphically embeddable into  $\mathcal{I}_1$ . To ensure that later, additional bookkeeping information is needed. Node labels are taken from the alphabet

$$\Gamma = \Gamma_0 \times 2^{\text{cl}(\mathcal{T}_1)} \times 2^{\text{CN}(\mathcal{T}_2)} \times \{0, 1\} \times 2^{\text{sub}(\mathcal{T}_2)},$$

where  $\Gamma_0$  is the set of all subsets of  $\Sigma_1 \cup \{R^- \mid R \in \Sigma_1\}$  that contain at most one role (a role name  $R$  or its inverse  $R^-$ ),  $\text{cl}(\mathcal{T}_i)$  is the set of subconcepts of (concepts in)  $\mathcal{T}_i$  closed under single negation, and  $\text{sub}(\mathcal{T}_2)$  is the set of subconcepts of (concepts in)  $\mathcal{T}_2$ . For a  $\Gamma$ -labeled tree  $(T, L)$  and a node  $x$  from  $T$ , we use  $L_i(x)$  to denote the  $(i+1)$ st component of  $L(x)$ , where  $i \in \{0, \dots, 4\}$ . Intuitively, the  $L_0$ -component represents the ABox  $\mathcal{A}$ , the  $L_1$ -component the model  $\mathcal{I}_1$ , the  $L_2$ -component represents  $\mathcal{I}_{\mathcal{T}_2, \mathcal{A}}$ , and the  $L_3$ - and  $L_4$ -components help to guarantee conditions (1) and (2) from Lemma 13.

To ensure that each component  $i \in \{0, \dots, 4\}$  indeed represents what it is supposed to, we impose on it an  *$i$ -properness* condition. For example, a  $\Gamma$ -labeled  $(T, L)$  tree is *0-proper* if (i)  $L_0(\varepsilon)$  contains no role and (ii) for every non-root node  $x$  of  $T$ ,  $L_0(x)$  contains a role. A 0-proper  $\Gamma$ -labeled tree  $(T, L)$  represents the following tree-shaped  $\Sigma_1$ -ABox:

$$\begin{aligned} \mathcal{A}_{(T, L)} = & \{A(x) \mid A \in L_0(x)\} \cup \\ & \{R(x, y) \mid R \in L_0(y), y \text{ is a child of } x\} \cup \\ & \{R(y, x) \mid R^- \in L_0(y), y \text{ is a child of } x\}. \end{aligned}$$

Due to space limitations, we skip the remaining definitions of properness and concentrate on explaining the most interesting components  $L_3$  and  $L_4$  of  $\Gamma$ -labels. The  $L_3$ -component marks a single node  $x$  in the tree, which is the individual  $a$  from Lemma 13 that satisfies conditions (1) and (2). If (1) is satisfied, we do not need the  $L_4$ -component. Otherwise, we store in that component at  $x$  a set of concepts  $S = \{\exists R.A, \forall R.B_1, \dots, \forall R.B_n\}$  such that  $R \in \Sigma_2$  and all concepts from  $S$  are true at  $x$  in  $\mathcal{I}_{\mathcal{T}_2, \mathcal{A}}$ . This *successor set* represents the  $R$ -successor  $d$  in condition (2) of Lemma 13. We then have to make sure that, for any neighboring node  $y$  of  $x$  that represents an  $R$ -successor of  $x$  in  $\mathcal{A}_{(T, L)}$ , we have  $(\mathcal{I}_{\mathcal{T}_2, \mathcal{A}}, d) \not\leq_{\Sigma_2} (\mathcal{I}_1, y)$ . This can again happen via a concept name or via a successor; we are done in the former case and use the  $L_4$ -component of  $y$  in the latter. It is important to note that we can never return to the same node in this tracing process since we only follow roles in the forward direction and the represented ABox is tree-shaped. This is crucial for achieving the EXPTIME overall complexity.

We show that  $\mathcal{T}_2$  is not  $\Theta$ -rCQ-entailed by  $\mathcal{T}_1$  iff there is an  $m$ -ary  $\Gamma$ -labeled tree that is  $i$ -proper for any  $i \in \{0, \dots, 4\}$ . It then remains to design a 2ABTA  $\mathfrak{A}$  that accepts exactly those

trees. We construct  $\mathfrak{A}$  as the intersection of five automata  $\mathfrak{A}_i$ ,  $i < 5$ , where each  $\mathfrak{A}_i$  ensures  $i$ -properness. Some of the automata are 2ABTAs with polynomially many states while others are NTAs with exponentially many states. We mix automata models since some properness conditions (2-properness) are much easier to describe with a 2ABTA while for others (4-properness), it does not seem to be possible to construct a 2ABTA with polynomially many states. In summary, we obtain the following result.

**Theorem 14.** *It is EXPTIME-complete to decide whether an  $\mathcal{ALC}$  TBox  $\mathcal{T}_1$  ( $\Sigma_1, \Sigma_2$ )-rCQ entails a Horn- $\mathcal{ALC}$  TBox  $\mathcal{T}_2$ .*

Note that the EXPTIME lower bound holds already for entailment of  $\mathcal{EL}$  TBoxes and  $\Sigma_1 = \Sigma_2$  [Lutz and Wolter, 2010]. We now study the non-rooted case, starting with an analogue of Theorem 12. As expected, moving to unrestricted queries corresponds to moving to unrestricted homomorphisms.

**Theorem 15.** *Let  $\mathcal{T}_1$  and  $\mathcal{T}_2$  be Horn- $\mathcal{ALC}$  TBoxes and  $\Theta = (\Sigma_1, \Sigma_2)$ . Then  $\mathcal{T}_1$   $\Theta$ -CQ entails  $\mathcal{T}_2$  iff, for all tree-shaped  $\Sigma_1$ -ABoxes  $\mathcal{A}$  of outdegree  $\leq |\mathcal{T}_2|$  and consistent with  $\mathcal{T}_1$  and  $\mathcal{T}_2$ ,  $\mathcal{I}_{\mathcal{T}_2, \mathcal{A}}$  is  $\Sigma_2$ -homomorphically embeddable into  $\mathcal{I}_{\mathcal{T}_1, \mathcal{A}}$ .*

The automata construction described above can largely be reused for this case. The main difference is that the two conditions in Lemma 13 need to be extended with a third one: there is an element  $d$  in the subtree of  $\mathcal{I}_{\mathcal{T}_2, \mathcal{A}}$  rooted at  $a$  that has an  $R$ -successor  $d_0$ ,  $R \notin \Sigma_2$ , such that, for all elements  $e$  of  $\mathcal{I}_1$ , we have  $(\mathcal{I}_2, d_0) \not\leq_{\Sigma_2} (\mathcal{I}_1, e)$ . To deal with this condition, it becomes necessary to store multiple successor sets in the  $L_4$ -components instead of only a single one, which increases the overall complexity to 2EXPTIME. A matching lower bound can be proved by a (non-trivial) reduction of the word problem for exponentially bounded alternating Turing machines.

**Theorem 16.**  *$\Theta$ -CQ entailment for Horn- $\mathcal{ALC}$  TBoxes is 2EXPTIME-complete. The lower bound holds for  $\Theta = (\Sigma, \Sigma)$ .*

## 7 Future Work

We have made first steps towards understanding query entailment and inseparability for KBs and TBoxes in expressive DLs. Many problems remain to be addressed. From a theoretical viewpoint, it would be of interest to solve the open problems in Figures 1 and 2, and also consider other expressive DLs such as *DL-Lite<sub>bool</sub><sup>H</sup>* [Artale et al., 2009] or *ALCI*. For example, if Theorem 10 could be generalized to UCQs (and  $\Sigma$ -homomorphisms), we would obtain a 2EXPTIME upper bound for UCQ-entailment between  $\mathcal{ALC}$  KBs using the same technique as for rUCQs. Also, our undecidability proof goes through for *DL-Lite<sub>bool</sub><sup>H</sup>*, but the other cases remain open. From a practical viewpoint, our model-theoretic criteria for query entailment are a good starting point for developing algorithms for approximations of query entailment based on simulations. Our undecidability and complexity results also indicate that rUCQ-entailment is more amenable to practical algorithms than, say, CQ-entailment and can be used as an approximation of the latter.

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