

# On Finite and Unrestricted Query Entailment beyond $SQ$ with Number Restrictions on Transitive Roles

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## Abstract

We study the description logic  $SQ$  with number restrictions applicable to transitive roles, extended with either *nominals* or *inverse roles*. We show tight 2EXPTIME upper bounds for *unrestricted* entailment of *regular path queries* for both extensions and *finite* entailment of *positive existential queries* for nominals. For inverses, we establish 2EXPTIME-completeness for *unrestricted* and *finite* entailment of *instance queries* (the latter under restriction to a single, transitive role).

## 1 Introduction

A prominent line of research in knowledge representation and database theory has focused on the evaluation of queries over incomplete data enriched by ontologies providing background knowledge. In this paradigm, ontologies are commonly formulated using description logics (DLs), believed to offer a good balance between expressivity and complexity. This is supported, for instance, by the good understanding of ‘data-tractable’ DLs [Kontchakov and Zakharyashev, 2014; Bienvenu and Ortiz, 2015]. Yet, for some expressive DLs the complexity of query entailment is less understood.

In this paper, we study query entailment in extensions of the description logic (DL)  $SQ$  allowing number restrictions ( $Q$ ) to be applied to transitive roles ( $S$ ). Most previous work on query entailment in expressive DLs, such as  $SHIQ$  or  $SHOQ$ , forbid the interaction of number restrictions and transitive roles [Glimm *et al.*, 2008b; Glimm *et al.*, 2008a; Calvanese *et al.*, 2014], but it is required in areas like biomedicine, e.g., to restrict the number of certain parts an organ has. For instance, one can express that the human heart has exactly one mitral valve, which has to be shared by its left and right atrium [Gutiérrez-Basulto *et al.*, 2018]. Allowing for the interaction of  $S$  and  $Q$  is dangerous in the sense that even modest extensions of  $SQ$ , such as with role inclusions or inverse roles, lead to an undecidable satisfiability problem [Kazakov *et al.*, 2007]. Decidability of satisfiability in  $SQ$  and in its extension with nominals was shown several years ago [Kazakov *et al.*, 2007;

Kaminski and Smolka, 2010], but only recently tight computational complexity bounds were established [Gutiérrez-Basulto *et al.*, 2017]. Even more recently, decidability for entailment of regular path queries over  $SQ$  knowledge bases was established. More precisely, based on a novel *tree-like model property* of  $SQ$  it was possible to devise an automata-based decision procedure yielding a tight 2EXPTIME upper bound [Gutiérrez-Basulto *et al.*, 2018].

The objective of this paper is to provide a more complete picture of query entailment in DLs with number restrictions on transitive roles. We pursue two specific goals.

First, we aim at understanding the limits of decidability of query entailment for such DLs. To this end, we investigate the extensions of  $SQ$  by *nominals* ( $SOQ$ ) and *controlled inverse roles* ( $SIQ^-$ ), where we allow number restrictions on inverse non-transitive roles and only existential restrictions on inverse transitive roles. As query language, we consider *positive existential regular path queries*, thus capturing the common languages of conjunctive and regular path queries.

Our second aim is to initiate the study of *finite* query entailment for  $SIQ^-$  and  $SOQ$ , where one is interested in reasoning only over finite models. This distinction is crucial because in database applications, both database instances and the models they represent are commonly assumed to be finite. The study of finite query entailment in  $SQ$  is interesting since, due to the presence of transitivity,  $SQ$  lacks *finite controllability*, and therefore unrestricted and finite entailment do not coincide. Interestingly, most previous works on finite query entailment consider logics lacking finite controllability because of number restrictions and inverse roles [Rosati, 2008; Pratt-Hartmann, 2009; Ibáñez-García *et al.*, 2014; Amarilli and Benedikt, 2015]. The study of finite query entailment in logics with transitivity (without number restrictions on transitive roles) started only recently [Rudolph, 2016; Gogacz *et al.*, 2018; Danielski and Kieronski, 2018]. Here, we focus on finite entailment of positive existential queries in  $SOQ$  and of instance queries in  $SIQ^-$ .

Our main contributions are as follows. In Sect. 3, we start by showing a *tree-like model property* for both  $SOQ$  and  $SIQ^-$ . More specifically, we carefully extend and adapt the *canonical* tree decompositions that were introduced for  $SQ$  in previous work [Gutiérrez-Basulto *et al.*, 2018] to also in-

corporate the presence of controlled inverses and nominals. Next, we prove that if a query is not entailed by a knowledge base (KB), then there is a counter-model with a canonical tree decomposition of small width. This tree-like model property is the basis for automata-based approaches to unrestricted and finite query entailment in the remainder of the paper. First, in Sect. 4, we construct tree automata to optimally decide entailment of regular path queries over  $SOQ$  and  $SIQ^-$  KBs in  $2EXPTIME$ . We move then, in Sect. 5, to finite entailment of positive existential queries over  $SOQ$  KBs, showing again an optimal  $2EXPTIME$  upper bound. To this end, we look at more refined canonical tree decompositions, which ensure the existence of a finite counter model. In other words, we reduce finite query entailment to entailment over models with this special canonical tree decomposition. Finally, in Sect. 6, we investigate the complexity for unrestricted and finite instance query (IQ) entailment in  $SIQ^-$ . In particular, we show that IQ entailment is  $2EXPTIME$ -hard both in the finite and in the unrestricted case. We found this surprising since it is rarely the case that IQ entailment becomes more difficult when inverses are added to the logic. Moreover, the result provides an orthogonal reason for  $2EXPTIME$ -hardness for conjunctive query entailment in  $SIQ^-$  [Lutz, 2008]. We complement this lower bound with matching upper bounds in the unrestricted case, thus confirming the conjecture that satisfiability in  $SIQ^-$  is decidable [Kazakov *et al.*, 2007]. In the finite case, we show a  $2EXPTIME$ -upper bound for KBs using a single transitive role. Note that  $SIQ^-$  with a single transitive role is a notational variant of the *graded modal logic with converse*  $\mathbf{K4}(\diamond_{\geq}, \diamond^-)$ . Thus, our result entails  $2EXPTIME$ -completeness for global consequence in  $\mathbf{K4}(\diamond_{\geq}, \diamond^-)$ , which was only known to be decidable [Bednarczyk *et al.*, 2019].

A long version with appendix can be found under <http://www.informatik.uni-bremen.de/tdki/research/papers.html>.

## 2 Preliminaries

### Description Logics

We consider a vocabulary consisting of countably infinite disjoint sets of *concept names*  $N_C$ , *role names*  $N_R$ , and *individual names*  $N_I$ , and assume that  $N_R$  is partitioned into two infinite sets of *non-transitive role names*  $N_R^{nt}$  and *transitive role names*  $N_R^t$ . A *role* is a role name or an *inverse role*  $r^-$ ; a *transitive role* is a transitive role name or the inverse of one.  $SIQ^-$ -concepts  $C, D$  are defined by the grammar

$$C, D ::= A \mid \neg C \mid C \sqcap D \mid \exists r.C \mid (\leq n s C)$$

where  $A \in N_C$ ,  $r$  is a role,  $n \geq 0$  is a natural number given in binary, and  $s$  is either a non-transitive role or a transitive role name.  $SOQ$ -concepts  $C, D$  are defined by the grammar

$$C, D ::= A \mid \neg C \mid C \sqcap D \mid \{a\} \mid (\leq n r C)$$

where  $A \in N_C$ ,  $r \in N_R$ ,  $a \in N_I$  and  $n$  is as above. We will use  $(\geq n r C)$  as abbreviation for  $\neg(\leq n-1 r C)$ , together with standard abbreviations  $\perp, \top, C \sqcup D, \forall r.C$ . Concepts of the form  $(\leq n r C)$ ,  $(\geq n r C)$ , and  $\{a\}$  are called *at-most restrictions*, *at-least restrictions*, and *nominals*, respectively. Note that in  $SIQ^-$  concepts, *inverse transitive roles* are not allowed in at-most and at-least restrictions.

A  $SIQ^-$ -TBox (respectively,  $SOQ$ -TBox)  $\mathcal{T}$  is a finite set of *concept inclusions (CIs)*  $C \sqsubseteq D$ , where  $C, D$  are  $SIQ^-$ -concepts (respectively,  $SOQ$ -concepts). An *ABox*  $\mathcal{A}$  is a finite non-empty set of *concept and role assertions* of the form  $A(a), r(a, b)$  where  $A \in N_C$ ,  $r \in N_R$  and  $\{a, b\} \subseteq N_I$ ;  $\text{ind}(\mathcal{A})$  is the set of individual names occurring in  $\mathcal{A}$ . A *knowledge base (KB)* is a pair  $\mathcal{K} = (\mathcal{T}, \mathcal{A})$ ;  $\text{nom}(\mathcal{K})$  is the set of nominals occurring in  $\mathcal{K}$  and  $\text{ind}(\mathcal{K}) = \text{ind}(\mathcal{A}) \cup \text{nom}(\mathcal{K})$ .

Without loss of generality, we assume throughout the paper that all CIs are in one of the following *normal forms*:

$$\begin{aligned} \prod_i A_i \sqsubseteq \bigsqcup_j B_j, \quad A \sqsubseteq \forall r^-.B, \quad A \sqsubseteq \exists r^-.B, \\ A \sqsubseteq (\leq n s B), \quad A \sqsubseteq (\geq n s B), \end{aligned}$$

where  $A, A_i, B, B_j$  are concept names or nominals,  $r \in N_R$ ,  $s$  is a non-transitive role or a transitive role name, and empty disjunction and conjunction are equivalent to  $\perp$  and  $\top$ , respectively. We further assume that for every at-most and at-least restriction,  $\mathcal{T}$  contains an equivalent concept name.

### Interpretations

The semantics is given as usual via *interpretations*  $\mathcal{I} = (\Delta^{\mathcal{I}}, \cdot^{\mathcal{I}})$  consisting of a non-empty *domain*  $\Delta^{\mathcal{I}}$  and an *interpretation function*  $\cdot^{\mathcal{I}}$  mapping concept names to subsets of the domain and role names to binary relations over the domain. Further, we adopt the *standard name assumption*, i.e.,  $a^{\mathcal{I}} = a$  for all  $a \in N_I$ . The interpretation of complex concepts  $C$  is defined in the usual way [Baader *et al.*, 2017]. An interpretation  $\mathcal{I}$  is a *model of a TBox*  $\mathcal{T}$ , written  $\mathcal{I} \models \mathcal{T}$  if  $C^{\mathcal{I}} \subseteq D^{\mathcal{I}}$  for all CIs  $C \sqsubseteq D \in \mathcal{T}$ . It is a *model of an ABox*  $\mathcal{A}$ , written  $\mathcal{I} \models \mathcal{A}$ , if  $(a, b) \in r^{\mathcal{I}}$  for all  $r(a, b) \in \mathcal{A}$  and  $a \in A^{\mathcal{I}}$  for all  $A(a) \in \mathcal{A}$ . Finally,  $\mathcal{I}$  is a *model of a KB*  $\mathcal{K} = (\mathcal{T}, \mathcal{A})$ , written  $\mathcal{I} \models \mathcal{K}$ , if  $\mathcal{I} \models \mathcal{T}$ ,  $\mathcal{I} \models \mathcal{A}$ , and  $r^{\mathcal{I}}$  is transitive for all  $r \in N_R^t$  occurring in  $\mathcal{K}$ . If  $\mathcal{K}$  has a model, we say that it is *satisfiable*.

An interpretation  $\mathcal{I}'$  is a *sub-interpretation* of  $\mathcal{I}$ , written as  $\mathcal{I}' \subseteq \mathcal{I}$ , if  $\Delta^{\mathcal{I}'} \subseteq \Delta^{\mathcal{I}}$ ,  $A^{\mathcal{I}'} \subseteq A^{\mathcal{I}}$ , and  $r^{\mathcal{I}'} \subseteq r^{\mathcal{I}}$  for all  $A \in N_C$  and  $r \in N_R$ . For  $\Sigma \subseteq N_C \cup N_R$ ,  $\mathcal{I}$  is a  $\Sigma$ -*interpretation* if  $A^{\mathcal{I}} = \emptyset$  and  $r^{\mathcal{I}} = \emptyset$  for all  $A \in N_C \setminus \Sigma$  and  $r \in N_R \setminus \Sigma$ . The *restriction of  $\mathcal{I}$  to signature  $\Sigma$*  is the maximal  $\Sigma$ -interpretation  $\mathcal{I}'$  with  $\mathcal{I}' \subseteq \mathcal{I}$ . The *restriction of  $\mathcal{I}$  to domain  $\Delta$*  is the maximal sub-interpretation of  $\mathcal{I}$  with domain  $\Delta$ . The union  $\mathcal{I} \cup \mathcal{J}$  of  $\mathcal{I}$  and  $\mathcal{J}$  is an interpretation such that  $\Delta^{\mathcal{I} \cup \mathcal{J}} = \Delta^{\mathcal{I}} \cup \Delta^{\mathcal{J}}$ ,  $A^{\mathcal{I} \cup \mathcal{J}} = A^{\mathcal{I}} \cup A^{\mathcal{J}}$ , and  $r^{\mathcal{I} \cup \mathcal{J}} = r^{\mathcal{I}} \cup r^{\mathcal{J}}$  for all  $A \in N_C$  and  $r \in N_R$ . The *transitive closure*  $\mathcal{I}^*$  of  $\mathcal{I}$  is an interpretation such that  $\Delta^{\mathcal{I}^*} = \Delta^{\mathcal{I}}$ ,  $A^{\mathcal{I}^*} = A^{\mathcal{I}}$  for all  $A \in N_C$ ,  $r^{\mathcal{I}^*} = r^{\mathcal{I}}$  for all  $r \in N_R^{nt}$ , and  $r^{\mathcal{I}^*} = (r^{\mathcal{I}})^+$  for all  $r \in N_R^t$ .

A *tree decomposition*  $\mathfrak{T}$  of an interpretation  $\mathcal{I}$  is a pair  $(T, \mathfrak{J})$  where  $T$  is a tree and  $\mathfrak{J}$  is a function that assigns an interpretation  $\mathfrak{J}(w) = (\Delta_w, \cdot^{\mathfrak{J}(w)})$  to each  $w \in T$  such that  $\mathcal{I} = \bigcup_{w \in T} \mathfrak{J}(w)$  and for every  $d \in \Delta^{\mathcal{I}}$ , the set  $\{w \in T \mid d \in \Delta_w\}$  is connected in  $T$ . We often blur the distinction between a node  $w$  of  $T$  and the associated interpretation  $\mathfrak{J}(w)$ , using the term *bag* for both. The *width* of  $\mathfrak{T}$  is  $\sup_{w \in T} |\Delta_w| - 1$ ; the *outdegree* of  $\mathfrak{T}$  is the outdegree of  $T$ . For each  $d \in \Delta^{\mathcal{I}}$ , there is a unique bag  $w$  closest to the root  $\varepsilon$  such that  $d \in \Delta_w$ . We say that  $d$  is *fresh* in this bag, and write  $F(w)$  for the set of all elements fresh in  $w$ .

## Ontology-mediated Query Entailment

A *positive existential regular path query (PRPQ)* is a first-order formula  $\varphi = \exists \mathbf{x} \psi(\mathbf{x})$  with  $\psi(\mathbf{x})$  constructed using  $\wedge$  and  $\vee$  over atoms of the form  $\mathcal{E}(t, t')$  where  $t, t'$  are variables from  $\mathbf{x}$  or individual names from  $\mathbb{N}_I$ , and  $\mathcal{E}$  is a *path expression* defined by the grammar

$$\mathcal{E}, \mathcal{E}' ::= r \mid r^- \mid A? \mid \mathcal{E}^* \mid \mathcal{E} \cup \mathcal{E}' \mid \mathcal{E} \circ \mathcal{E}',$$

where  $r \in \mathbb{N}_R$  and  $A \in \mathbb{N}_C$ . A PEQ is a PRPQ that does not use the operators  $*$ ,  $\cup$ , and  $\circ$  in path expressions. Equivalently, it is an FO formula  $\varphi = \exists \mathbf{x} \psi(\mathbf{x})$  where  $\psi$  is constructed using  $\wedge$  and  $\vee$  over atoms  $r(t, t')$  and  $A(t')$  with  $t, t'$  as above. An *instance query (IQ)* is just an expression of the shape  $C(a)$  for some concept  $C$  and  $a \in \mathbb{N}_I$ .

The semantics of PRPQs is defined via matches. Let us fix a PRPQ  $\varphi = \exists \mathbf{x} \psi(\mathbf{x})$  and an interpretation  $\mathcal{I}$ . Let  $\text{ind}(\varphi)$  be the set of individual names in  $\varphi$ . A *match for  $\varphi$  in  $\mathcal{I}$*  is a function  $\pi : \mathbf{x} \cup \text{ind}(\varphi) \rightarrow \Delta^{\mathcal{I}}$  such that  $\pi(a) = a$ , for all  $a \in \text{ind}(\varphi)$ , and  $\mathcal{I}, \pi \models \psi(\mathbf{x})$  under the standard semantics of first-order logic extended with a rule for atoms of the form  $\mathcal{E}(t, t')$ . An interpretation  $\mathcal{I}$  satisfies  $\varphi$ , written as  $\mathcal{I} \models \varphi$ , if there is a match for  $\varphi$  in  $\mathcal{I}$ .

A PRPQ  $\varphi$  is (*finitely*) *entailed by a KB  $\mathcal{K}$* , if  $\mathcal{I} \models \varphi$  for every (finite) model  $\mathcal{I}$  of  $\mathcal{K}$ ; we write  $\mathcal{K} \models \varphi$  and  $\mathcal{K} \models_{\text{fin}} \varphi$ , respectively, in this case. Accordingly, we write  $\mathcal{K} \models C(a)$  and  $\mathcal{K} \models_{\text{fin}} C(a)$  if  $a \in C^{\mathcal{I}}$  in all (finite) models  $\mathcal{I}$  of  $\mathcal{K}$ .

We study the corresponding *decision problem*—whether a given query is (finitely) entailed by a given KB—for different choices of knowledge base and query languages.

## 3 Tree-like Counter-Model Property

In this section we show a tree-like model property for  $SIQ^-$  and  $SOQ$ : we show that if a query is not entailed by a KB, then there is a counter-model with a tree decomposition of bounded width and outdegree. For the automata-based decision procedure to yield optimal upper bounds, it is useful to consider *canonical decompositions* which we define next.

In canonical decompositions elements will be accompanied by certain key neighbors. Let us fix a KB  $\mathcal{K} = (\mathcal{T}, \mathcal{A})$ . For an interpretation  $\mathcal{I}$ , an element  $d \in \Delta^{\mathcal{I}}$ , and  $r \in \mathbb{N}_R^t$ , the  *$r$ -cluster of  $d$  in  $\mathcal{I}$* , denoted by  $Q_r^{\mathcal{I}}(d)$ , is the set containing  $d$  and each  $e \in \Delta^{\mathcal{I}}$  such that both  $(d, e) \in r^{\mathcal{I}}$  and  $(e, d) \in r^{\mathcal{I}}$ . This is the closest environment of  $d$  wrt.  $r$ . We also associate with  $d$  a larger set  $\text{rel}_r^{\mathcal{I}}(d)$  of  $r$ -successors *relevant for the at-most restrictions of  $\mathcal{K}$* . We let  $\text{rel}_r^{\mathcal{I}}(d)$  be the least set  $X$  such that  $Q_r^{\mathcal{I}}(d) \subseteq X$  and for all  $e \in X$ ,  $f \in \Delta^{\mathcal{I}}$ , and  $A \sqsubseteq (\leq n r B)$  in  $\mathcal{T}$ , if  $e \in A^{\mathcal{I}}$ ,  $f \in B^{\mathcal{I}}$ , and  $(e, f) \in r^{\mathcal{I}*}$ , then  $Q_r^{\mathcal{I}}(f) \subseteq X$ . The construction of canonical decompositions relies on the following properties of relevant successors.

**Lemma 1.** *For each  $r \in \mathbb{N}_R^t$ , the following hold:*

1. *for all  $d, e \in \Delta^{\mathcal{I}}$ , if  $e \in \text{rel}_r^{\mathcal{I}}(d)$  then  $\text{rel}_r^{\mathcal{I}}(e) \subseteq \text{rel}_r^{\mathcal{I}}(d)$ ;*
2. *if each  $r$ -cluster in  $\mathcal{I}$  has size at most  $N$ , then for each  $d \in \Delta^{\mathcal{I}}$ ,  $|\text{rel}_r^{\mathcal{I}}(d)| \leq N \cdot 2^{\text{poly}(|\mathcal{T}|)}$ .*

In a canonical tree decomposition, formalized in Definition 1 below, each non-root bag keeps track of all concepts and a single role indicated by  $\tau$ . Nominals are captured

within a finite subinterpretation  $\mathcal{M}$  represented faithfully in all bags; in the absence of nominals, one can take empty  $\mathcal{M}$  and drop (C<sub>4</sub>). Conditions (C<sub>0</sub>)–(C<sub>3</sub>) ensure that apart from  $\Delta^{\mathcal{M}}$ , neighboring non-root bags share a single element, sometimes accompanied by its relevant successors.

**Definition 1.** *A tree decomposition  $\mathfrak{T} = (T, \mathfrak{J})$  is canonical if there exists  $\tau : T \rightarrow \mathbb{N}_R \cup \{\perp\}$  with  $\tau^{-1}(\perp) = \{\varepsilon\}$  such that*

- (B<sub>0</sub>) *for each  $w \in T$ ,  $\mathfrak{J}(w)$  is a  $\Sigma_w$ -interpretation where  $\Sigma_\varepsilon = \mathbb{N}_C \cup \mathbb{N}_R^t$  and  $\Sigma_w = \mathbb{N}_C \cup \{\tau(w)\}$  for  $w \neq \varepsilon$ ;*
  - (B<sub>1</sub>) *for all  $v, w \in T$ , the restrictions of  $\mathfrak{J}(v)$  and  $\mathfrak{J}(w)$  to domain  $\Delta_v \cap \Delta_w$  and signature  $\Sigma_v \cap \Sigma_w$  coincide;*
  - (B<sub>2</sub>) *for each  $v \in T \setminus \{\varepsilon\}$ ,  $d \in F(v)$ , and  $r \in \mathbb{N}_R^t \setminus \{\tau(v)\}$ , a unique child  $w$  of  $v$  satisfies  $\tau(w) = r$  and  $d \in \Delta_w$ ;*
- and there is an interpretation  $\mathcal{M}$  with  $\text{nom}(\mathcal{K}) \subseteq \Delta^{\mathcal{M}} \subseteq \Delta_\varepsilon$ , such that for each  $w \in T \setminus \{\varepsilon\}$  and its parent  $v$ , one has*
- (C<sub>0</sub>) *if  $\tau(w) \in \mathbb{N}_R^t$  and  $v = \varepsilon$ , then  $\Delta_\varepsilon \subseteq \Delta_w$ ;*
  - (C<sub>1</sub>) *if  $\tau(w) \in \mathbb{N}_R^t$ , then  $\Delta_v \cap \Delta_w = \{d\} \cup \Delta^{\mathcal{M}}$  for some  $d \in F(v)$ ;*
  - (C<sub>2</sub>) *if  $\tau(v) \neq \tau(w) \in \mathbb{N}_R^t$  and  $v \neq \varepsilon$ , then  $\Delta_w \cap \Delta_v = \{d\} \cup \Delta^{\mathcal{M}}$  for some  $d \in F(v)$ ;*
  - (C<sub>3</sub>) *if  $\tau(w) = \tau(v) = r \in \mathbb{N}_R^t$ , then  $\Delta_v \cap \Delta_w = \text{rel}_r^{\mathfrak{J}(v)}(d) \cup \Delta^{\mathcal{M}}$  and  $\text{rel}_r^{\mathfrak{J}(v)}(d) = \text{rel}_r^{\mathfrak{J}(w)}(d)$  for some  $d$  such that either  $d \in F(v)$  or  $d \in F(u)$  and  $\tau(u) \neq \tau(v)$  for the parent  $u$  of  $v$ ; and*
  - (C<sub>4</sub>) *if  $\tau(w) = r \in \mathbb{N}_R^t$ , then  $\text{rel}_r^{\mathfrak{J}(w)}(d) = \text{rel}_r^{\mathcal{M}}(d)$  for all  $d \in \Delta^{\mathcal{M}}$ .*

**Theorem 1.** *Let  $\mathcal{K} = (\mathcal{T}, \mathcal{A})$  be a KB in normal form and  $\varphi$  a PRPQ with  $\mathcal{K} \not\models \varphi$ . If  $\mathcal{K}$  is a  $SOQ$  KB or a  $SIQ^-$  KB, then there exists a model  $\mathcal{J}$  of  $\mathcal{T}$  and  $\mathcal{A}$  such that*

- *$\mathcal{J}$  has a canonical tree decomposition of width and out-degree  $\text{poly}(|\text{ind}(\mathcal{K})|) \cdot 2^{\text{poly}(|\mathcal{T}|)}$ ; and*
- *$\mathcal{J}^* \models \mathcal{K}$  and  $\mathcal{J}^* \not\models \varphi$ .*<sup>1</sup>

*Proof.* Let us fix a counter-model  $\mathcal{I}$  for  $\mathcal{K}$  and  $\varphi$ . We can assume that  $|Q_r^{\mathcal{I}}(d)| \leq |\text{ind}(\mathcal{K})| + 2^{\text{poly}(|\mathcal{T}|)}$  for all  $d \in \Delta^{\mathcal{I}}$  [Gutiérrez-Basulto *et al.*, 2018]. By Lemma 1,  $|\text{rel}_r^{\mathcal{I}}(d)| \leq |\text{ind}(\mathcal{K})| \cdot 2^{\text{poly}(|\mathcal{T}|)}$  for all  $d \in \Delta^{\mathcal{I}}$ .

To build a canonical tree decomposition  $\mathfrak{T}$ , we unravel  $\mathcal{I}$  starting from the interpretation of the ABox and then applying the extension rules (R<sub>0</sub>)–(R<sub>3</sub>) below, corresponding to conditions (C<sub>0</sub>)–(C<sub>3</sub>): (R<sub>0</sub>) collects relevant successors of the individuals in the ABox, (R<sub>1</sub>) performs standard unraveling of non-transitive roles, (R<sub>2</sub>) takes care of the change of roles, and (R<sub>3</sub>) realizes further unraveling of transitive roles.

More precisely, for the root bag, we take  $\mathcal{I}$  restricted to the domain  $\text{ind}(\mathcal{A}) \cup \Delta$  and the signature  $\mathbb{N}_C \cup \mathbb{N}_R^t$ , where  $\Delta$  is the union of  $\text{rel}_r^{\mathcal{I}}(a)$  for all  $a \in \text{nom}(\mathcal{K})$  and  $r \in \mathbb{N}_R^t$ .

(R<sub>0</sub>) For each  $r \in \mathbb{N}_R^t$ , we add as a child bag of  $\varepsilon$  the restriction of  $\mathcal{I}$  to signature  $\mathbb{N}_C \cup \{r\}$  and domain  $\bigcup_{a \in \text{ind}(\mathcal{A})} \text{rel}_r^{\mathcal{I}}(a) \cup \Delta$  with each  $e \notin \text{ind}(\mathcal{A}) \cup \Delta$  replaced by a fresh copy  $e'$ . We call  $e$  the *original of  $e'$* .

<sup>1</sup>Recall that in a model of the ABox or the TBox, the extensions of role names from  $\mathbb{N}_R^t$  need not be transitive.

Then, we use the following rules  $(\mathbf{R}_1)$ – $(\mathbf{R}_3)$  *ad infinitum*, applying each rule only once to each previously added bag  $v$ .

$(\mathbf{R}_1)$  For each  $r \in \mathbb{N}_R^{nt}$ , and each  $d' \in F(v)$ , let  $d \in \Delta^{\mathcal{I}}$  be the original of  $d'$  (possibly  $d = d'$ ) and let  $W_0$  be the set of originals of all  $r$ -successors and  $r$ -predecessors of  $d'$  in  $\mathcal{I}(v)$ . Pick a minimal set  $W \subseteq \Delta^{\mathcal{I}}$  containing  $\{d\} \cup W_0 \cup \Delta$  such that for each  $s \in \{r, r^-\}$  and  $A \sqsubseteq (\geq n s B)$  in  $\mathcal{T}$ , if  $d \in A^{\mathcal{I}}$ , then  $d$  has at least  $n$  different  $s$ -successors in  $B^{\mathcal{I}} \cap W$ . For each  $e \in W \setminus (W_0 \setminus \Delta)$ , add as a child bag of  $v$  the restriction of  $\mathcal{I}$  to signature  $\mathbb{N}_C \cup \{r\}$  and domain  $\{d, e\} \cup \Delta$  with all  $r$ -edges from  $\Delta \setminus \{d\}$  to  $\{d, e\} \setminus \Delta$  removed,  $d$  replaced by  $d'$  and each  $f \in \{e\} \setminus \Delta$ , by a fresh copy  $f'$ .

$(\mathbf{R}_2)$  Assuming  $v \neq \varepsilon$ , for each  $r \in \mathbb{N}_R^t$  with  $r \neq \tau(v)$ , and each  $d' \in F(v)$ , let  $d$  be the original of  $d'$ . Add as a child bag of  $v$  the restriction of  $\mathcal{I}$  to signature  $\mathbb{N}_C \cup \{r\}$  and domain  $\text{rel}_r^{\mathcal{I}}(d) \cup \Delta$  where  $d$  is replaced by  $d'$  and each  $e \in \text{rel}_r^{\mathcal{I}}(d) \setminus (\{d\} \cup \Delta)$ , by a fresh copy  $e'$ .

$(\mathbf{R}_3)$  Assuming  $\tau(v) = r \in \mathbb{N}_R^t$ , for each  $d' \in \Delta^v$  fresh in  $v$  or in the parent  $u$  of  $v$  with  $\tau(u) \neq r$ , let  $d$  be the original of  $d'$ . Pick a minimal set  $W \subseteq \Delta^{\mathcal{I}}$  containing  $\text{rel}_r^{\mathcal{I}}(d) \cup \Delta$  such that for each  $A \sqsubseteq (\geq n r B)$  in  $\mathcal{T}$ , if  $d \in A^{\mathcal{I}}$ , then  $d$  has at least  $n$  different  $r$ -successors in  $B^{\mathcal{I}} \cap W$ , and for each  $A \sqsubseteq \exists r^-.B$  in  $\mathcal{T}$ , if  $d \in A^{\mathcal{I}}$ , then  $d$  has an  $r^-$ -successor in  $B^{\mathcal{I}} \cap W$ . For each  $e \in W \setminus (\text{rel}_r^{\mathcal{I}}(d) \cup \Delta)$ , add as a child bag of  $v$  the restriction of  $\mathcal{I}$  to the signature  $\mathbb{N}_C \cup \{r\}$  and domain  $\text{rel}_r^{\mathcal{I}}(e) \cup \text{rel}_r^{\mathcal{I}}(d) \cup \Delta$  where each element  $f \in \text{rel}_r^{\mathcal{I}}(d) \setminus \Delta$  is replaced by its copy  $f'$  from  $\mathcal{I}(v)$ , and each element  $f \in \text{rel}_r^{\mathcal{I}}(e) \setminus (\text{rel}_r^{\mathcal{I}}(d) \cup \Delta)$  by a fresh copy  $f'$ .

Let  $\mathcal{J}$  be the interpretation underlying the resulting decomposition  $\mathfrak{T}$ . The function mapping each  $d' \in \Delta^{\mathcal{J}}$  to its original  $d \in \Delta^{\mathcal{I}}$  gives a homomorphism from  $\mathcal{J}$  to  $\mathcal{I}$ , and consequently also from  $\mathcal{J}^*$  to  $\mathcal{I}$ . It follows that  $\mathcal{J}^* \not\models \varphi$ . Taking  $\mathcal{I}$  restricted to  $\Delta$  as  $\mathcal{M}$ , it is routine to check that  $\mathfrak{T}$  and  $\mathcal{J}$  satisfy the remaining postulated properties. Note that while the construction is described for any normalized  $\mathcal{K}$ ,  $(\mathbf{R}_1)$  is correct only if  $\mathcal{K}$  is either a  $SOQ$  KB or a  $SIQ^-$  KB. Correctness of  $(\mathbf{R}_2)$  and  $(\mathbf{R}_3)$  follows from Lemma 1 (1).  $\square$

## 4 PRPQ Entailment for $SIQ^-$ and $SOQ$

We shall now exploit canonicity of tree decompositions in an automata-based decision procedure for query entailment in  $SIQ^-$  and  $SOQ$ , yielding optimal complexity upper bounds.

Let us fix a  $(SIQ^-$  or  $SOQ)$  KB  $\mathcal{K}$  and a PRPQ  $\varphi$ , and denote with  $\Sigma_C, \Sigma_R^t, \Sigma_R^{nt}$  the concept names, transitive role names, and non-transitive role names used in  $\mathcal{K}$ . By Theorem 1, if  $\varphi$  is not entailed by  $\mathcal{K}$ , there exists a counter-model admitting a canonical tree decomposition of width and outdegree bounded by a constant  $N$  single exponential in  $|\mathcal{K}|$ . We effectively construct a non-deterministic tree automaton recognizing such decompositions of counter-models, and thus reduce query entailment to the emptiness problem.

Let us introduce the necessary notions for tree automata. A  $k$ -ary  $\Omega$ -labeled tree is a pair  $(T, \tau)$  where  $T$  is a tree each of whose nodes has at most  $k$  successors and  $\tau : T \rightarrow \Omega$  assigns a letter from  $\Omega$  to each node. A *non-deterministic tree automaton (NTA)* over  $k$ -ary  $\Omega$ -labeled trees is a tuple  $\mathfrak{A} = (Q, \Omega, q_0, \Lambda)$ , where  $Q$  is a finite set of states,  $q_0 \in Q$  is the initial state,  $\Lambda \subseteq \bigcup_{i \leq k} (Q \times \Omega \times Q^i)$  is a

set of transitions. A *run*  $r$  on a  $k$ -ary  $\Omega$ -labeled tree  $(T, \tau)$  is a  $Q$ -labeled tree  $(T, r)$  such that  $r(\varepsilon) = q_0$  and, for every  $x \in T$  with successors  $x_1, \dots, x_m$ , there is a transition  $(r(x), \tau(x), r(x_1) \cdots r(x_m)) \in \Lambda$ . As usual,  $\mathfrak{A}$  *recognizes* the set of all  $\Omega$ -labeled trees admitting a run.

Since counter-models have a potentially infinite domain, we *encode* tree decompositions of width  $N$  using a domain  $D$  of  $2N$  elements, similar to what has been done, e.g., in [Grädel and Walukiewicz, 1999]. Intuitively, if  $w$  is a successor node of  $v$  in the tree decomposition, then an element  $d$  occurring in (the bag at)  $w$  represents a fresh domain element iff  $d$  does not occur in  $v$ . More precisely, the alphabet  $\Omega$  of the automaton is the set of all pairs  $(x, \mathcal{I})$  such that either  $x \in \Sigma_R$  and  $\mathcal{I}$  is a  $\Sigma_C \cup \{x\}$ -interpretation with  $\Delta^{\mathcal{I}} \subseteq D$ , or  $x = \perp$  and  $\mathcal{I}$  is a  $\Sigma_C \cup \Sigma_R^{nt}$ -interpretation with  $\Delta^{\mathcal{I}} \subseteq D$ .

**Lemma 2.** *Given  $\mathcal{K}$ ,  $\varphi$ , and  $N$ , one can compute in time  $O(2^{\text{poly}(N)})$  an NTA recognizing the set of encodings of canonical tree decompositions of width and outdegree at most  $N$  such that for the underlying interpretation  $\mathcal{J}$  it holds that  $\mathcal{J}^* \models \mathcal{K}$  and  $\mathcal{J}^* \not\models \varphi$ , as well as  $\mathcal{J} \models \mathcal{A}$  and  $\mathcal{J} \models \mathcal{T}$ .*

*Proof.* The desired NTA is the intersection of an NTA  $\mathfrak{A}_{\mathcal{K}}$  recognizing all canonical tree decompositions such that the underlying interpretation  $\mathcal{J}$  satisfies  $\mathcal{J} \models \mathcal{A}$ ,  $\mathcal{J} \models \mathcal{T}$ , and  $\mathcal{J}^* \models \mathcal{K}$  and an NTA  $\mathfrak{A}_{\neg\varphi}$  recognizing all tree decompositions of counter-models of  $\varphi$ . Since the latter is known from [Gutiérrez-Basulto *et al.*, 2018, Lemma 6], we concentrate on  $\mathfrak{A}_{\mathcal{K}} = (Q, \Omega, q_0, \Lambda)$ , working over  $N$ -ary trees.

Informally, its construction relies on the following ideas: (i) by  $(\mathbf{B}_2)$  and  $(\mathbf{C}_2)$ , in every bag there is at most one  $d$  satisfying the condition ‘ $d \in F(u) \dots$ ’ in Condition  $(\mathbf{C}_3)$ ; thus, (ii) canonicity can be checked by initially guessing  $\mathcal{M}$  and then comparing neighboring interpretations and remembering the mentioned  $d$  in the states; (iii)  $\mathcal{J} \models \mathcal{A}$  can be verified by looking at labels of the root and its direct successors; (iv) due to canonicity and the TBox normal form,  $\mathcal{J} \models \mathcal{T}$  can be verified by looking at the current label (this suffices for at-most restrictions over transitive roles, due to canonicity) and possibly at successor bags (at-least restrictions, and at-most restrictions over non-transitive roles); (v)  $\mathcal{J}^* \models \mathcal{T}$  is a consequence of  $\mathcal{J} \models \mathcal{T}$ , by the normal form.

Formally, the set  $Q$  contains  $q_0$  and all tuples of the shape

$$\langle (x, \mathcal{I}), F, \mathcal{M}, \mathcal{B}, \mathcal{C}, e, r, f \rangle,$$

where  $(x, \mathcal{I}) \in \Omega$ ,  $F \subseteq \Delta^{\mathcal{I}}$ ,  $\mathcal{M}$  is a  $\Sigma_C \cup \Sigma_R^{nt}$ -interpretation with  $\Delta^{\mathcal{M}} \subseteq D$ ,  $\mathcal{B} \subseteq \mathcal{A}$ ,  $\mathcal{C}$  is a set of assertions of the shape  $(\geq n s B)(d)$ ,  $(\leq n s B)(d)$ , or  $(\exists s.B)(d)$  with  $d \in D$ ,  $B \in \Sigma_C$ ,  $s$  a role in  $\mathcal{T}$ ,  $n \leq N$ , and  $e, f \in D \cup \{\varepsilon\}$ ,  $r \in \Sigma_R^t$ .

In state  $q = \langle (x, \mathcal{I}), F, \mathcal{M}, \mathcal{B}, \mathcal{C}, e, r, f \rangle$  reading symbol  $a = (x', \mathcal{I}')$ , the automaton allows a transition only in case the following conditions are satisfied:

- Conditions  $(\mathbf{B}_0)$ – $(\mathbf{B}_2)$  and  $(\mathbf{C}_0)$ – $(\mathbf{C}_4)$  with  $\mathcal{I}, \mathcal{I}', x, x', F$  taking the role of  $\mathcal{I}(v), \mathcal{I}(w), \tau(v), \tau(w), F(v)$ , respectively, and ‘ $d \in F(u) \dots$ ’ in  $(\mathbf{C}_3)$  replaced with ‘ $d = f'$ ’;
- $x' \neq \perp$  and, if  $x = \perp$ , then  $\mathcal{I}' \models \mathcal{B}$ ;
- either  $e \neq \varepsilon$ ,  $e \in \Delta^{\mathcal{I}'}$ , and  $r = x'$ , or  $e = \varepsilon$  and  $x = x'$ ;
- $\mathcal{I}' \models C(d)$  for all  $C(d) \in \mathcal{C}$  with  $d \in \Delta^{\mathcal{I}'}$  or  $C$  of shape  $(\geq n s B)$  or  $\exists r^-.B$ ;

- $\mathcal{I}' \models \alpha$  for all  $\alpha \in \mathcal{T}$  of the form  $\prod_i A_i \sqsubseteq \prod_j B_j$ ,  $A \sqsubseteq (\leq n r B)$ , and  $A \sqsubseteq \forall r^- . B$ .

In this case,  $\Lambda$  allows all transitions  $(q, a, q_1 \cdots q_m)$ ,  $m \leq N$  where each  $q_i$  is of shape  $\langle (x', \mathcal{I}'), F', \mathcal{M}, \emptyset, \mathcal{C}_i, e_i, r_i, f_i \rangle$  with  $F' = \Delta^{\mathcal{I}'} \setminus \Delta^{\mathcal{I}}$  and:

- for each  $d \in F'$  and each  $r \in \Sigma_R^t \setminus \{x'\}$ , there is a unique  $i$  such that  $e_i = d$  and  $r_i = r$ ; conversely, if  $e_i \neq \varepsilon$  for some  $i$ , then  $e_i \in F'$  and  $r_i \neq x'$ ;
- if  $e \neq \varepsilon$ , then  $f_i = e$ , for all  $i$ ;
- for all  $A \sqsubseteq \exists r^- . B \in \mathcal{T}$  and  $d \in A^{\mathcal{I}'} \cap F'$  such that  $d \notin (\exists r^- . B)^{\mathcal{I}'}$ , we have  $(\exists r^- . B)(d) \in \mathcal{B}_i$  for some  $i$ ;
- for all  $A \sqsubseteq (\leq n r B) \in \mathcal{T}$ ,  $r \in \Sigma_R^{nt}$ , and  $d \in A^{\mathcal{I}'} \cap F'$ , there is a partition  $n = n_0 + \dots + n_m$ , such that  $d \in (\leq n_0 r B)^{\mathcal{I}'}$ , and  $(\leq n_i r B)(d) \in \mathcal{C}_i$ , for all  $i$ ;
- for all  $A \sqsubseteq (\geq n s B) \in \mathcal{T}$  and  $d \in A^{\mathcal{I}'} \cap F'$ , there is a partition  $n = n_0 + \dots + n_m$ , such that  $d \in (\geq n_0 s B)^{\mathcal{I}'}$  and  $(\geq n_i s B)(d) \in \mathcal{C}_i$ , for all  $i$  with  $n_i > 0$ .

The transitions for  $q_0$  are similar, but they additionally nondeterministically initialize  $\mathcal{M}$  and check the non-transitive part of the ABox in the root, see the appendix. Correctness of the automaton is essentially a consequence of Points (i)–(v) mentioned above. It is routine to verify that  $\mathfrak{A}_{\mathcal{K}}$  is of the required size and can be constructed in the required time.  $\square$

Recall that emptiness of NTAs can be checked in polynomial time. Thus, Lemma 2 together with the bounds on  $N$  from Theorem 1, yields a 2EXPTIME upper bound for PRPQ entailment in  $SIQ^-$  and  $SOQ$ . A matching lower bound is inherited from positive existential query answering in  $\mathcal{ALC}$  [Calvanese *et al.*, 2014].

**Theorem 2.** *PRPQ entailment over  $SIQ^-$  and  $SOQ$  knowledge bases is 2EXPTIME-complete.*

## 5 Finite PEQ Entailment for $SOQ$

The goal of this section is to establish the following result.

**Theorem 3.** *Finite PEQ entailment over  $SOQ$  knowledge bases is 2EXPTIME-complete.*

The lower bound follows directly from the result on unrestricted query entailment for  $\mathcal{ALCO}$  [Ngo *et al.*, 2016], as the latter logic enjoys finite controllability. For the upper bound, we carefully adapt an approach previously used for  $SCF$  [Gogacz *et al.*, 2018], which relies on the following additional condition imposed on tree-like counter-models.

**Definition 2.** *A canonical tree decomposition is safe, if it contains no infinite downward path such that for each node  $w$  in this path,  $\tau(w)$  is the same transitive role name.*

In what follows, by a *counter-witness* we understand a model of the ABox and the TBox whose transitive closure is a counter-model. The approach requires two ingredients: (1) equivalence of the existence of a finite counter-model and the existence of a counter-witness that admits a safe canonical tree decomposition, and (2) effective regularity of the set of safe canonical tree decompositions (of given width and outdegree) of counter-witnesses. For (2), observe that safety can be

easily checked by an automaton with Büchi acceptance condition [Grädel *et al.*, 2002] and the number of states quadratic in the number of transitive role names in  $\mathcal{K}$ : on each path the automaton remembers the role names associated with two most recently visited nodes; the state is accepting unless they are the same transitive role name. The product of this automaton and the one constructed in the previous section recognizes the desired language. Assuming (1) is also available, the upper bound follows like for the unrestricted case: the algorithm builds the automaton and tests its emptiness.

The remainder of this section provides (1). One implication is obtained via the following observation.

**Lemma 3.** *If  $\mathcal{I}$  is a finite interpretation of a  $SOQ$  KB, then the unravelling procedure from the proof of Theorem 1 yields a safe tree decomposition.*

To prove the converse implication we begin from a carefully chosen counter-witness with a safe canonical tree decomposition. It is well known that each regular set of trees contains a *regular tree*, i.e., a tree with finitely many non-isomorphic subtrees. Hence, if there is a counter-witness with a safe canonical tree decomposition, there is also one with a regular safe canonical tree decomposition. Let  $\mathfrak{T} = (T, \mathfrak{J})$  be such a tree decomposition of some counter-witness  $\mathcal{I}$ , and let  $\mathcal{M}$  be the interpretation guaranteed by Definition 1.

Let us restructure  $\mathfrak{T}$  by iteratively merging neighboring nodes associated to the same transitive role name: pick a node  $v$  with a child  $w$  such that  $\tau(v) = \tau(w) \in N_R^t$ , redefine  $\mathfrak{J}(v)$  as  $\mathfrak{J}(v) \cup \mathfrak{J}(w)$ , remove  $w$  from  $\mathfrak{T}$ , and promote all children of  $w$  to children of  $v$ . As a result we obtain a canonical tree decomposition  $\mathfrak{S} = (S, \mathfrak{J})$  of  $\mathcal{I}$ . By construction,  $\mathfrak{S}$  is *strongly canonical*: no neighboring nodes in  $\mathfrak{S}$  are associated with the same transitive role name. Hence, for each node  $w$  with parent  $v \neq \varepsilon$ ,  $\Delta_v \cap \Delta_w \setminus \Delta^{\mathcal{M}} = \{d_w\}$  for some  $d_w \in F(v)$ .

Each regular safe tree decomposition has bounded length of downward paths of nodes associated with the same transitive role name. Consequently, the restructuring above keeps the outdegree and the width bounded.

**Lemma 4.**  *$\mathfrak{S}$  has bounded degree and width.*

We can now easily turn  $\mathcal{I}^*$  into a finite model of  $\mathcal{K}$ . Suppose that on each path of  $\mathfrak{S}$ , we fix a node  $v$  and its ancestor  $u$  (neither  $\varepsilon$  nor a child of  $\varepsilon$ ) such that  $\tau(v) = \tau(u)$ ,  $\mathfrak{J}(v) \simeq \mathfrak{J}(u)$ , and the witnessing isomorphism  $h$  maps  $d_v$  to  $d_u$  and is identity over  $\Delta^{\mathcal{M}}$ . Suppose also that for each element in  $\Delta^{\mathcal{M}}$ , all witnesses required by at-least restrictions can be found among elements of  $\Delta^{\mathcal{M}}$  and elements that do not occur in the subtrees of  $\mathfrak{S}$  rooted at the chosen nodes  $v$ . Note that for each path we can find such a pair of nodes, because the sizes of the bags are bounded in  $\mathfrak{S}$ . We shall modify  $\mathcal{I}$  by removing parts of it and redirecting edges previously leading to the removed parts. Pick any path such that the corresponding  $d_v$  has not been processed yet and has not been removed. Remove from  $\mathcal{I}$  the union of  $\Delta_w$  with  $w$  ranging over descendants of  $v$  (including  $v$ ), keeping only  $\Delta^{\mathcal{M}}$  and  $d_v$ . Replace each  $\tau(v)$ -edge leading from  $d_v$  to a removed element  $e \in \Delta_v$ , with an  $\tau(v)$ -edge leading from  $d_v$  to  $h(e)$ . Repeat until no such path exists. The resulting interpretation  $\mathcal{J}$  is obviously finite. Checking correctness is routine.

**Lemma 5.**  $\mathcal{J}^* \models \mathcal{K}$ .

To ensure that  $\mathcal{J}^* \not\models \varphi$  we need to choose the nodes  $v$  and  $u$  more carefully. Relying on  $\varphi$  being a PEQ, not an arbitrary PRPQ, we apply the colored blocking principle [Gogacz *et al.*, 2018]: to keep  $u$  and  $v$  sufficiently similar and sufficiently far apart, we look at their neighborhoods of sufficiently large radius and use additional coloring to distinguish elements within each neighborhood (see Appendix for details).

## 6 IQ Entailment

We also get the following results on IQ entailment.

**Theorem 4.** *Finite and unrestricted IQ entailment is CONEXPTIME-complete over  $\mathcal{SOQ}$  KBs. Unrestricted IQ entailment over  $\mathcal{SIQ}^-$  KBs and finite IQ entailment over  $\mathcal{SIQ}^-$  KBs restricted to a single transitive role and no non-transitive roles is 2EXPTIME-complete.*

*Proof.* As is well-known, (finite) IQ entailment reduces to the complement of (finite) KB satisfiability; we focus on the latter. For  $\mathcal{SOQ}$ , we simply use the facts that (finite) KB satisfiability for  $\mathcal{SOQ}$  is NEXPTIME-complete [Gutiérrez-Basulto *et al.*, 2017] and that the lower bound holds in the finite [Kazakov and Pratt-Hartmann, 2009].

The 2EXPTIME upper bound for unrestricted KB satisfiability follows from Theorem 2, and for finite satisfiability in the above fragment of  $\mathcal{SIQ}^-$  follows from Theorem 2 and a recent result by Bednarczyk *et al.* [2019], implying that satisfiability and finite satisfiability coincide for this fragment of  $\mathcal{SIQ}^-$ . This approach cannot be generalized to full  $\mathcal{SIQ}^-$  since  $\mathcal{SIQ}^-$  lacks the finite model property.

We next show that these upper bounds are tight by reducing the word problem for  $2^n$ -space bounded *alternating Turing machines (ATMs)*, which is known to be 2EXPTIME-hard [Chandra *et al.*, 1981]. An ATM  $M = (Q, \Theta, \Gamma, q_0, \Delta)$  consists of the set  $Q$  of states partitioned into *existential states*  $Q_{\exists}$  and *universal states*  $Q_{\forall}$ , the input alphabet  $\Theta$ , the tape alphabet  $\Gamma$ , the *starting state*  $q_0 \in Q_{\exists}$ , and the *transition relation*  $\Delta$ . Without loss of generality, we assume that each of  $M$ 's configurations has exactly two successor configurations, universal and existential states alternate, and  $M$  accepts a word iff there is an infinite (alternating) run.

Given  $M, w$ , we construct in polynomial time a knowledge base  $\mathcal{K} = (\mathcal{T}, \{I(a_0)\})$  using a single transitive role name  $r$  such that  $M$  accepts  $w$  iff  $\mathcal{K}$  is satisfiable. We represent configurations of size  $2^n$  in the leaves of binary trees of depth  $n$ . To this end, we use concept names  $X_0, \dots, X_{n-1}$  (representing bits of an exponential counter) and  $L_0, \dots, L_n$  (for the levels of the tree), and include the following CIs for all  $i, j$  with  $0 \leq i < n$  and  $i < j \leq n$ :

$$\begin{aligned} L_i &\sqsubseteq \exists r.(X_i \sqcap L_{i+1}) \sqcap \exists r.(\neg X_i \sqcap L_{i+1}) \\ L_{i+1} \sqcap X_i &\sqsubseteq \forall r.(L_j \rightarrow X_i) \\ L_{i+1} \sqcap \neg X_i &\sqsubseteq \forall r.(L_j \rightarrow \neg X_i) \end{aligned}$$

It should be clear that every model of  $L_0$  and these CIs contains a full binary tree of depth  $n$  such that the *leaves*, that is, the elements satisfying  $L_n$ , correspond to the numbers  $0, \dots, 2^n - 1$  in the natural way, via concept names  $X_i$ . Let  $\Sigma = \Gamma \cup (Q \times \Gamma)$  be the set of possible labels of a cell in

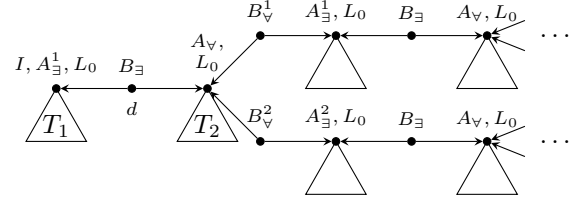
$M$ 's computation, and introduce concept names  $C_{\sigma}^x$  for every  $\sigma \in \Sigma$ ,  $x \in \{l, h, r\}$ . Every leaf with number  $i$  is labeled with three concepts  $C_{\sigma_1}^l, C_{\sigma_2}^h, C_{\sigma_3}^r$  representing the cells  $i-1, i, i+1$  of a configuration using the CI:

$$L_n \sqsubseteq \prod_{x \in \{l, h, r\}} \bigsqcup_{\sigma \in \Sigma} (C_{\sigma}^x \sqcap \prod_{\sigma' \neq \sigma} \neg C_{\sigma'}^x)$$

We use these trees as follows. The concept name  $I$  enforces a skeleton structure modeling an alternating computation using the following CIs, for  $i \in \{1, 2\}$ :

$$\begin{aligned} I &\sqsubseteq A_{\exists}^1 & A_{\exists}^i &\sqsubseteq L_0 \sqcap \exists r^-.(B_{\exists} \sqcap \exists r.A_{\forall}^i) \\ & & A_{\forall} &\sqsubseteq L_0 \sqcap \exists r^-.(B_{\forall}^i \sqcap \exists r.A_{\exists}^i) \end{aligned}$$

Thus, every model of  $I$  contains the following structure, where every triangle represents one of the described trees, and  $A_{\forall}(A_{\exists}^i)$  marks universal (existential) configurations:



It remains to ensure that (i) the leaf labeling in every tree is actually a configuration, (ii) neighboring trees describe successor configurations, and (iii) the first tree is labeled with the initial configuration. We concentrate on (ii), as (i) is similar and (iii) is straightforward. We illustrate the idea on  $T_1$  and  $T_2$  in the figure. In  $T_1$ , we enforce in every leaf an  $r$ -successor satisfying the label of that cell in the successor configuration (computable from the  $C_{\sigma}^x$ ). In  $T_2$ , we enforce in every leaf an  $r$ -successor with the current label  $C_{\sigma}^h$ . Both in  $T_1$  and  $T_2$ , these additional elements satisfy a fresh concept name  $S$  and have the same counter value as in the leaves. Observe that, by transitivity, all  $2 \cdot 2^n$  created nodes are ‘visible’ from  $d$  satisfying  $B_{\exists}$  in the figure. By including the CI  $B_{\exists} \sqsubseteq (\leq 2^n r S)$ ,  $S$ -elements with the same counter value from  $T_1$  and  $T_2$  are forced to identify, thus achieving the desired synchronization. Having (i)–(iii) in place, it is routine to show that  $\mathcal{K}$  is satisfiable iff  $M$  accepts  $w$ . The lower bound applies to finite satisfiability, since  $\mathcal{K}$  is satisfiable iff it is finitely satisfiable.  $\square$

## 7 Outlook

This paper makes a step towards a complete picture of query entailment in DLs with number restrictions on transitive roles. There are several natural next steps involving finite entailment. The first is to cover full  $\mathcal{SIQ}^-$ . A more challenging goal is to go beyond instance queries: an immediate obstacle is that the natural safety condition for  $\mathcal{SIQ}^-$  does not guarantee strongly canonical decompositions. Covering full PRPQs even just for  $\mathcal{SQ}$  seems to require generalizing the colored blocking principle, or finding an entirely different tool.

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## A Additional Preliminaries

We define the semantics of PRPQs as follows:

- $\mathcal{I}, \pi \models \psi_1 \vee \psi_2$  iff  $\mathcal{I}, \pi \models \psi_1$  or  $\mathcal{I}, \pi \models \psi_2$ ;
- $\mathcal{I}, \pi \models \psi_1 \wedge \psi_2$  iff  $\mathcal{I}, \pi \models \psi_1$  and  $\mathcal{I}, \pi \models \psi_2$ ;
- $\mathcal{I}, \pi \models \mathcal{E}(t, t')$  iff  $(\pi(t), \pi(t')) \in \mathcal{E}^{\mathcal{I}}$ , with  $\mathcal{E}^{\mathcal{I}}$  defined as follows:

$$\begin{aligned} (r^-)^{\mathcal{I}} &= \{(e, d) \mid (d, e) \in r^{\mathcal{I}}\} \\ (A?)^{\mathcal{I}} &= \{(d, d) \mid d \in A^{\mathcal{I}}\} \\ (\mathcal{E}^*)^{\mathcal{I}} &= (\mathcal{E}^{\mathcal{I}})^* \\ (\mathcal{E} \cup \mathcal{E}')^{\mathcal{I}} &= \mathcal{E}^{\mathcal{I}} \cup \mathcal{E}'^{\mathcal{I}} \\ (\mathcal{E} \circ \mathcal{E}')^{\mathcal{I}} &= \mathcal{E}^{\mathcal{I}} \circ \mathcal{E}'^{\mathcal{I}} \end{aligned}$$

A *tree* is a prefix-closed subset  $T \subseteq (\mathbb{N} \setminus \{0\})^*$ . A node  $w \in T$  is a *successor* of  $v \in T$  and  $v$  is a *predecessor* of  $w$  if  $w = v \cdot i$  for some  $i \in \mathbb{N}$ . We say that the node  $\varepsilon$  is the *root* of  $T$ .

A (*non-deterministic*) *tree automaton* with *Büchi acceptance condition* is a tree automaton enriched with a set of accepting states  $F \subseteq Q$ . A run of such an automaton is considered accepting if on each branch accepting states occur infinitely often.

### Normal Form

As stated in the main part of the paper we assume normalized KBs, such that each CIs in the TBox takes one of the following forms:

$$\begin{aligned} \prod_i A_i \sqsubseteq \prod_j B_j, \quad A \sqsubseteq \forall r^- . B, \quad A \sqsubseteq \exists r^- . B, \\ A \sqsubseteq (\leq n s B), \quad A \sqsubseteq (\geq n s B), \end{aligned}$$

where  $A, A_i, B, B_j$  are concept names or nominals,  $r \in \mathbb{N}_R$ ,  $s$  is a non-transitive role or a transitive role name, and empty disjunction and conjunction are equivalent to  $\perp$  and  $\top$ , respectively. This can be assumed w.l.o.g. since every  $SIQ^-$  or  $SOQ$  TBox can be transformed into a normalized one by extending its signature with an appropriate number (linear on the size of the TBox) of fresh concept names. We further assume that for every at-most restriction  $(\leq n s B)$ ,  $\mathcal{T}$  also contains the following

$$A \sqsubseteq (\leq n s B), \quad A' \sqsubseteq (\geq n + 1 s B), \quad \top \sqsubseteq A \sqcup A' \quad (1)$$

with  $A$  a concept name, not occurring on the left-hand-side of any other CI. We make an analogous assumption for at-least restrictions.

## B Additional Proofs for Section 3

**Lemma 1.** *For each  $r \in \mathbb{N}_R^+$ , the following hold:*

1. for all  $d, e \in \Delta^{\mathcal{I}}$ , if  $e \in \text{rel}_r^{\mathcal{I}}(d)$  then  $\text{rel}_r^{\mathcal{I}}(e) \subseteq \text{rel}_r^{\mathcal{I}}(d)$ ;
2. if each  $r$ -cluster in  $\mathcal{I}$  has size at most  $N$ , then for each  $d \in \Delta^{\mathcal{I}}$ ,  $|\text{rel}_r^{\mathcal{I}}(d)| \leq N \cdot 2^{\text{poly}(|\mathcal{T}|)}$ .

*Proof.* Point 1 is a consequence of the definition of  $\text{rel}_r^{\mathcal{I}}(d)$ .

For Point 2, let us denote with  $\text{atm}(\mathcal{T})$  the set of all at-most restrictions occurring in  $\mathcal{T}$ . We say that  $e \in \Delta^{\mathcal{I}}$  is *directly relevant* for  $d \in \Delta^{\mathcal{I}}$  if there is some  $(\leq n r B) \in \mathcal{T}$ , such that  $d \in (\leq n r B)^{\mathcal{I}}$ ,  $e \in B^{\mathcal{I}}$ , and  $(d, e) \in r^{\mathcal{I}}$ . We further denote with  $X_r^{\mathcal{I}}(d)$  the smallest set that contains  $d$  and is closed under direct relevant elements. Because  $\mathcal{I} \models \mathcal{T}$ , we have

$$\text{rel}_r^{\mathcal{I}}(d) \subseteq \bigcup_{e \in X_r^{\mathcal{I}}(d)} Q_r^{\mathcal{I}}(e).$$

It thus suffices to prove that the size of  $X_r^{\mathcal{I}}$  is bounded by  $2^{\text{poly}(|\mathcal{T}|)}$ .

To see this, consider the directed tree  $(V, E)$  with  $V = X_r^{\mathcal{I}}(d)$  and  $E$  is defined as follows. Start with setting  $E$  the set of all  $(d, e)$  such that  $e$  is directly relevant for  $d$  and apply the following step exhaustively.

- (\*) Choose leaf  $e \in V$  and add, for all  $f \in \Delta^{\mathcal{I}}$  directly relevant for  $e$ , but not for any of  $e$ 's predecessors an edge  $(e, f)$  to  $E$ .

By definition of  $V$  and direct relevance,  $(V, E)$  is a connected tree. Now, consider the labelling  $\ell : V \rightarrow 2^{\text{atm}(\mathcal{T})}$  given by

$$\ell(e) = \{C \mid e \in (\leq n r C)^{\mathcal{I}}, (\leq n r C) \in \text{atm}(\mathcal{T})\}.$$

Let  $(e, f) \in E$ . By construction, we have

- $\ell(e) \subseteq \ell(f)$  if  $f$  is a leaf in  $(V, E)$ , and
- $\ell(e) \subsetneq \ell(f)$  if  $f$  is an inner node in  $(V, E)$ .

Thus, the depth of the tree  $(V, E)$  is bounded by  $|\mathcal{T}|$ . Observe moreover that also the outdegree of  $(V, E)$  is bounded exponentially in  $\mathcal{T}$  by definition of direct relevance. Overall, we get that the size of  $V = X_r^{\mathcal{I}}(d)$  is bounded by an exponential in  $\mathcal{T}$ .  $\square$

**Theorem 1.** *Let  $\mathcal{K} = (\mathcal{T}, \mathcal{A})$  be a KB in normal form and  $\varphi$  a PRPQ with  $\mathcal{K} \not\models \varphi$ . If  $\mathcal{K}$  is a  $SOQ$  KB or a  $SIQ^-$  KB, then there exists a model  $\mathcal{J}$  of  $\mathcal{T}$  and  $\mathcal{A}$  such that*

- $\mathcal{J}$  has a canonical tree decomposition of width and out-degree  $\text{poly}(|\text{ind}(\mathcal{K})|) \cdot 2^{\text{poly}(|\mathcal{T}|)}$ ; and
- $\mathcal{J}^* \models \mathcal{K}$  and  $\mathcal{J}^* \not\models \varphi$ .<sup>2</sup>

The construction of the decomposition  $\mathfrak{T}$  described in the body of the paper directly ensures that  $\mathfrak{T}$  is a canonical decomposition of width and outdegree appropriately bounded. It remains to check that the interpretation  $\mathcal{J}$  underlying the decomposition  $\mathfrak{T}$  satisfies the conditions required in the statement of the theorem.

**Claim 1.**  $\mathcal{J} \models (\mathcal{T}, \mathcal{A})$

*Proof.* During the proof, we will repeatedly use the following fact, a consequence of the existence of a homomorphism from  $\mathcal{J}$  to  $\mathcal{I}$ .

- (†) The unary type of each element  $d'$  in  $\mathcal{J}$  coincides with that of its original  $d$  in  $\mathcal{I}$ .

<sup>2</sup>Recall that in a model of the ABox or the TBox, the extensions of role names from  $\mathbb{N}_R^+$  need not be transitive.



All the assertions in  $\mathcal{A}$  are satisfied in  $\mathcal{J}$  since the root bag in the tree decomposition of  $\mathcal{J}$  contains all the individuals in  $\mathcal{A}$ , as well as all the non-transitive edges involving those elements, and because all edges of transitive roles among individuals are added by  $(\mathbf{R}_0)$ .

If  $\mathcal{K}$  is a  $\mathcal{SOQ}$  KB, the construction of  $\mathcal{J}$  ensures that each nominal is interpreted by a singleton. Indeed, since every bag in the tree decomposition contains the set of elements  $\Delta$ , consisting of all the nominals and their relevant  $r$ -successors for every transitive role  $r$ , the definition of the root bag and rules  $(\mathbf{R}_0) - (\mathbf{R}_3)$  ensure that for every role name edges between elements in  $\mathcal{I}$  and  $\Delta$  are faithfully replicated in  $\mathcal{J}$ .

Next, we need to show that for every CI  $C \sqsubseteq D \in \mathcal{T}$  it holds that  $C^{\mathcal{J}} \subseteq D^{\mathcal{J}}$ . For the case where  $D$  is of the form  $\bigsqcup_j B_j$ , this follows directly from  $(\dagger)$ . For the case where  $D$  is a universal, existential, at-most or at-least restriction over a non-transitive role, the statement holds by construction because of  $(\mathbf{R}_1)$ . It thus remains to consider restrictions involving transitive roles. Assume that  $r$  is a transitive role name and let  $f' \in C^{\mathcal{J}}$ .

If  $D = \exists r^-.B$  or  $D = (\geq n r B)$  for some concept name  $B$ , then  $(\mathbf{R}_3)$  ensures that  $f' \in D^{\mathcal{I}}$ , whereas for the case where  $D = \forall r^-.B$ , this follows since  $B$  is a concept name and because of  $(\dagger)$ . Indeed, assume  $(e', f') \in r^{\mathcal{J}}$ , and let  $e$  be the original of  $e'$ . By construction,  $\mathcal{J}$  can be mapped homomorphically to  $\mathcal{I}$ , and thus we have  $(e, f) \in r^{\mathcal{I}}$ . Because the unary types of  $f$  and  $f'$  coincide, and  $\mathcal{I} \models \mathcal{K}$ , it holds that  $e \in B^{\mathcal{I}}$  and therefore  $e' \in B^{\mathcal{J}}$ .

The case where  $D = (\leq n r B)$  is slightly more subtle. Let  $f$  be the original of  $f'$  in  $\mathcal{I}$ . We shall need a subclaim that during the construction of  $\mathcal{J}$  exactly one copy of each element from  $\text{rel}_r^{\mathcal{I}}(f)$  was introduced among  $r$ -successors of  $f'$ . Let  $w$  be the bag closest to the root bag containing  $f'$  and such that  $\text{r}(w) = r$ . Let us see that  $w$  contains exactly one copy of each element from  $\text{rel}_r^{\mathcal{I}}(f)$ . Indeed,  $w$  could have only been introduced by  $(\mathbf{R}_0)$ ,  $(\mathbf{R}_2)$  or  $(\mathbf{R}_3)$ .

If  $w$  was introduced by  $(\mathbf{R}_2)$ , using point 1 of Lemma 1 we see immediately that  $\text{rel}_r^{\mathcal{I}}(f) \subseteq \text{rel}_r^{\mathcal{I}}(d)$ , where  $d$  is like in the formulation of rule  $(\mathbf{R}_2)$ , and so it is clear that  $\mathcal{J}(w)$  contains exactly one copy of each element from  $\text{rel}_r^{\mathcal{I}}(f)$ .

For  $w$  introduced by  $(\mathbf{R}_0)$ , the argument is analogous.

Now assume  $w$  was introduced by  $(\mathbf{R}_3)$ . Let  $v$  be the parent of  $w$  and let  $d'$  and  $d$  be like in the formulation of rule  $(\mathbf{R}_3)$ . Then,  $f'$  is a copy of an element  $f$  from  $\text{rel}_r^{\mathcal{I}}(e)$ , where  $e$  is an  $r$ -successor (or  $r^-$ -successor) of  $d$  and  $e \notin \text{rel}_r^{\mathcal{I}}(d) \cup \Delta$ . By point 1 of Lemma 1,  $\text{rel}_r^{\mathcal{I}}(f) \subseteq \text{rel}_r^{\mathcal{I}}(e)$ . Hence, the rule adds exactly one copy of each element of  $\text{rel}_r^{\mathcal{I}}(f)$ : either a fresh copy, or the copy inherited from  $v$  if the element belongs to  $\text{rel}_r^{\mathcal{I}}(d) \cup \Delta$ .

Every other possible  $r$ -successor of  $f'$  can only be added by a subsequent application of  $(\mathbf{R}_3)$ . The definition of this rule ensures that each fresh element added in this way is a copy of an  $r$ -successor of  $f$  that does not belong to  $\text{rel}_r^{\mathcal{I}}(f)$ . This completes the proof of the subclaim.

Now, assume that  $f' \in C^{\mathcal{J}}$ . Because  $\mathcal{J}$  maps homomorphically into  $\mathcal{I}$ , if  $g'$  is an  $r$ -successor of  $f'$  that belongs to  $B^{\mathcal{J}}$ , then its original  $g$  is an  $r$ -successor of  $f$  that belongs to

$B^{\mathcal{I}}$ . We also know that  $f \in C^{\mathcal{I}}$  and because  $\mathcal{I} \models \mathcal{T}$  we know that there is at most  $n$  such elements  $g$  and they all belong to  $\text{rel}_r^{\mathcal{I}}(f)$ . But elements of  $\text{rel}_r^{\mathcal{I}}(f)$  are copied exactly once among  $r$ -successors of  $f'$ , so the number of possible  $g'$  is also bounded by  $n$ , and we are done.  $\square$

**Claim 2.**  $\mathcal{J}^* \models \mathcal{K}$

*Proof.* Clearly, by definition of  $\mathcal{J}^*$ , every transitive role is interpreted as a transitive relation.

Now, we observe that the homomorphism from  $\mathcal{J}$  to  $\mathcal{I}$  can be naturally extended to a homomorphism from  $\mathcal{J}^*$  to  $\mathcal{I}$ . Thus,  $(\dagger)$  applies also to the unary types of elements in  $\mathcal{J}^*$ . Therefore,  $\mathcal{J} \models (\mathcal{T}, \mathcal{A})$  implies that  $\mathcal{J}^* \models \mathcal{A}$ , and that  $\mathcal{J}^*$  satisfies every concept inclusion  $C \sqsubseteq D$ , for every  $D$  of the form  $\prod_j B_j, \exists r^-.B$  with  $r$  a role name, and  $(\geq n s B)$  with  $s$  a non-transitive role or a transitive role name. It remains to deal with universal and at-most restrictions. For  $D = \forall r^-.B$ , the argument is the same as for  $\mathcal{J}$ .

To show that  $\mathcal{J}^*$  satisfies CIs of the form  $C \sqsubseteq (\leq n r B)$ , with  $r$  a transitive role name, we use the subclaim used in the proof for  $\mathcal{J}$ . Let  $f' \in C^{\mathcal{J}^*}$  and  $w$  be the bag closest to the root such that  $f' \in F(w)$  and  $\text{r}(w) = r$ . We will show that no fresh  $r$ -successors of  $f'$  (in  $\mathcal{J}^*$ ) violating the at-most restriction are added as a result of multiple applications of rule  $(\mathbf{R}_3)$ . More precisely, we show that for every  $g' \in B^{\mathcal{J}^*}$ , if  $(f', g') \in r^{\mathcal{J}^*}$ , then  $g' \in \Delta_w$ .

Towards a contradiction, suppose that at some point among those successors one fresh element  $g'$  is added, such that  $g' \in B^{\mathcal{J}}$ . Then there exists a path of bags  $w = w_0, w_1, w_2, \dots, w_k$  with  $k > 0$ , corresponding to  $r$ -successors  $f' = e'_0, e'_1, e'_2, \dots, e'_k = g'$  and their originals  $f = e_0, e_1, e_2, \dots, e_k = g$ , such that  $e'_k \in F(w_k)$ . Since  $\mathcal{K}$  is normalized, (1) ensures that there is a concept name  $A$  that is equivalent to  $(\leq n r B)$ . Because  $\mathcal{I} \models \mathcal{K}$ , we have  $f \in A^{\mathcal{I}}$ ; it then follows by  $(\dagger)$  that  $f' \in A^{\mathcal{J}}$ . Furthermore,  $(f, e_{k-1}) \in r^{\mathcal{I}}$ , implies  $e_{k-1} \in (\leq n r B)^{\mathcal{I}}$  and therefore  $e_{k-1} \in A^{\mathcal{I}}$ . Since  $e_k \in B^{\mathcal{I}}$ , it then follows that  $e_k \in \text{rel}_r^{\mathcal{I}}(e_{k-1})$ . However, this contradicts the assumption that  $e'_k \in F(w_k)$ , because by the subclaim, there is exactly one copy of every relevant successor of  $e_{k-1}$  in  $\Delta_{k-1}$ , and the definition of  $(\mathbf{R}_3)$  prevents the introduction of fresh copies of these elements.  $\square$

## C Missing proofs for Section 4

### Encoding Tree Decompositions

We provide missing details on the encoding. Let  $(T, \tau)$  be a  $\Omega$ -labeled tree with  $\Omega$  defined as in the main part. For convenience, we use  $\mathcal{I}_w$  and  $r_w$  to refer to the single components of  $\tau$  in a node  $w$ , that is,  $\tau(w) = (r_w, \mathcal{I}_w)$ . Given an element  $d \in \Delta$ , we say that  $v, w \in T$  are  $d$ -connected iff  $d \in \Delta^{\mathcal{I}_u}$  for all  $u$  on the unique shortest path from  $v$  to  $w$ . In case  $d \in \Delta^{\mathcal{I}_w}$ , we use  $[w]_d$  to denote the set of all  $v$  which are  $d$ -connected to  $w$ . We call  $(T, \tau)$   $\mathcal{A}$ -consistent if  $\text{ind}(\mathcal{A}) \subseteq \Delta^{\mathcal{I}_e}$ . An  $\mathcal{A}$ -consistent  $\Omega$ -labeled tree  $(T, \tau)$  represents a pair  $(T, \mathcal{J})$  where the interpretations  $\mathcal{J}(w)$  are defined by taking, for all  $w \in T$ :

$$\Delta_w = \{[w]_d \mid d \in \Delta^{\mathcal{I}_w}\},$$

$$A^{\mathcal{J}(w)} = \{[w]_d \mid d \in A^{\mathcal{I}^w}\},$$

$$r^{\mathcal{J}(w)} = \{([w]_d, [w]_e) \mid (d, e) \in r^{\mathcal{I}^w}\},$$

for all concept names  $A$  and role names  $r$  occurring in  $\mathcal{K}$ . We further associate an interpretation  $\mathcal{I}_{(T,\tau)}$  to every consistent  $\Omega$ -labeled tree by taking  $\mathcal{I}_{(T,\tau)} = \bigcup_{w \in T} \mathcal{J}(w)$  and interpret individual names  $a \in \text{ind}(\mathcal{A})$  by taking  $a^{\mathcal{I}_{(T,\tau)}} = [\varepsilon]_a$ . Note that this is well-defined due to  $\mathcal{A}$ -consistency. It can be easily verified that  $(T, \mathcal{J})$  is a tree decomposition of  $\mathcal{I}_{(T,\tau)}$ . Conversely, given some interpretation  $\mathcal{I}$  and a tree decomposition  $(T, \mathcal{J})$  of  $\mathcal{I}$  of width  $K$ , one can construct a  $\mathcal{A}$ -consistent  $(T, \tau)$  such that  $\mathcal{I}_{(T,\tau)}$  is isomorphic to  $\mathcal{I}$ , based on the size  $2K$  of  $\Delta$  [Grädel and Walukiewicz, 1999]. Note that in both cases the outdegree is preserved so that it suffices to consider  $N$ -ary trees throughout.

**Lemma 2.** *Given  $\mathcal{K}$ ,  $\varphi$ , and  $N$ , one can compute in time  $O(2^{\text{poly}(N)})$  an NTA recognizing the set of encodings of canonical tree decompositions of width and outdegree at most  $N$  such that for the underlying interpretation  $\mathcal{J}$  it holds that  $\mathcal{J}^* \models \mathcal{K}$  and  $\mathcal{J}^* \not\models \varphi$ , as well as  $\mathcal{J} \models \mathcal{A}$  and  $\mathcal{J} \models \mathcal{T}$ .*

We provide the missing transitions for the initial state  $q_0$  on input symbol  $(x, \mathcal{I})$ . The automaton allows transitions only in case  $x = \perp$ ,  $\text{ind}(\mathcal{A}) \subseteq \Delta^{\mathcal{I}}$ , and  $\mathcal{I} \models \mathcal{A}^{nt}$  where  $\mathcal{A}^{nt}$  is obtained from  $\mathcal{A}$  by dropping all assertions  $r(a, b)$  with  $r$  a transitive role. In such a case,  $\Lambda$  contains all transitions  $(q_0, (x, \mathcal{I}), q_1 \cdots q_m)$ ,  $m \leq N$  where  $q_i$  is of shape  $\langle (x, \mathcal{I}), F', \mathcal{M}, \mathcal{B}_i, \mathcal{C}_i, e_i, r_i, f_i \rangle$  with  $F' = \Delta^{\mathcal{I}}$  and  $\mathcal{M}$  some  $\Sigma_{\mathcal{C}} \cup \Sigma_{\mathcal{R}}^{nt}$ -interpretation with  $\Delta^{\mathcal{M}} \subseteq \Delta^{\mathcal{I}}$  such that the five conditions from the main part are satisfied and additionally  $A = \mathcal{A}^{nt} \cup \bigcup_i \mathcal{B}_i$ .

## D Missing proofs for Section 5

**Lemma 3.** *If  $\mathcal{I}$  is a finite interpretation of a SOQ KB, then the unravelling procedure from the proof of Theorem 1 yields a safe tree decomposition.*

*Proof.* Let  $w$  be a child of a node  $v$  with  $\tau(w) = \tau(v) = r$  for some  $r \in \mathbb{N}_{\mathcal{R}}^t$ . Then,  $w$  was added to the tree decomposition by applying the rule  $(\mathbf{R}_3)$ . Let  $e$  and  $d$  be as in  $(\mathbf{R}_3)$ . Because we are working with a SOQ KB,  $e$  is an  $r$ -successor of  $d$ . We can also conclude that there is no  $r$ -path from  $e$  to  $d$ , because otherwise we would have  $e \in Q_r^{\mathcal{I}}(d) \subseteq \text{rel}_r^{\mathcal{I}}(d)$ , which is explicitly excluded in  $(\mathbf{R}_3)$ . It follows that the length of any path of nodes  $u$  with  $\tau(u) = r$  is bounded by the number of  $r$ -clusters in  $\mathcal{I}$ , which is finite.  $\square$

**Lemma 4.**  $\mathfrak{S}$  has bounded degree and width.

*Proof.*  $\mathfrak{T}$  is regular, so it has at most  $p$  non-isomorphic subtrees for some  $p \in \mathbb{N}$ .

Consider a downward path of nodes in  $\mathfrak{T}$  associated with the same transitive role  $r$ . If this path is longer than  $p$ , the subtrees rooted at some two nodes on this path are isomorphic. Because one of them is a proper subtree of the other, it follows immediately that  $\mathfrak{T}$  contains an infinite downward path of nodes associated with  $r$ , which contradicts safety. Consequently, such a path has length at most  $p$ .

Consider a connected subset of nodes of  $\mathfrak{T}$  associated with a transitive role name  $r$ . It is necessarily a subtree of  $\mathfrak{T}$ . By the argument above, the height of this tree is at most  $p$ . Because  $\mathfrak{T}$  has bounded outdegree, the size of the subtree is bounded.

It follows that each interpretation assigned to a node of  $\mathfrak{S}$  is the union of a bounded number of interpretations of bounded size. Hence,  $\mathfrak{S}$  has bounded width.

Similarly, the outdegree of any node of  $\mathfrak{S}$  is the sum of the outdegrees of a bounded number of nodes of  $\mathfrak{T}$ . Hence,  $\mathfrak{S}$  has bounded outdegree.  $\square$

## Coloured Blocking Principle

We first recall (and adapt) key definitions and technical results underlying colored blocking Gogacz *et al.*. The difference wrt. to the original is that the set of elements that need to be excluded from the interpretation to make it well-behaved is now  $\Delta^{\mathcal{M}}$ , not just  $\text{nom}(\mathcal{K})$ . This does not affect the cited results. The whole development is entirely independent of the knowledge base, and works for any finite set of excluded elements. The only property of nominals that is ever used is that they are preserved by homomorphisms. Thus, in what follows all homomorphisms (and consequently all isomorphisms) are assumed to be identity over  $\Delta^{\mathcal{M}}$ . We shall write  $\mathcal{I} \setminus \Delta^{\mathcal{M}}$  for the interpretation  $\mathcal{I}$  restricted to the domain  $\Delta^{\mathcal{I}} \setminus \Delta^{\mathcal{M}}$ .

**Definition 3.** *For  $d \in \Delta^{\mathcal{I}} \setminus \Delta^{\mathcal{M}}$ , the  $n$ -neighbourhood  $N_n^{\mathcal{I}}(d)$  is the subinterpretation of  $\mathcal{I}$  induced by  $\Delta^{\mathcal{M}}$  and all elements  $e \in \Delta^{\mathcal{I}} \setminus \Delta^{\mathcal{M}}$  within distance  $n$  from  $d$  in  $\mathcal{I} \setminus \Delta^{\mathcal{M}}$ , enriched with a fresh concept interpreted as  $\{d\}$ . For  $a \in \Delta^{\mathcal{M}}$ ,  $N_n^{\mathcal{I}}(a)$  is the subinterpretation induced by  $\Delta^{\mathcal{M}}$ , enriched similarly.*

**Definition 4.** *A coloring with  $k$  colors of an interpretation  $\mathcal{I}$  is any interpretation  $\mathcal{I}'$  that enriches  $\mathcal{I}$  with  $k$  fresh concept names  $B_1, \dots, B_k$ , provided that  $B_1^{\mathcal{I}'}, \dots, B_k^{\mathcal{I}'}$  is a partition of  $\Delta^{\mathcal{I}'}$ . We say that  $d \in B_i^{\mathcal{I}'}$  has color  $B_i$ . A coloring  $\mathcal{I}'$  is  $n$ -proper if for each  $d \in \Delta^{\mathcal{I}'}$  all elements of  $N_n^{\mathcal{I}'}(d)$  have different colors.*

**Lemma 6.** *If  $\mathcal{I} \setminus \Delta^{\mathcal{M}}$  has bounded degree, then for all  $n \geq 0$  there exists an  $n$ -proper coloring of  $\mathcal{I}$  with finitely many colors.*

**Definition 5.** *An interpretation  $\mathcal{I}$  is  $\ell$ -bounded if for each  $r \in \mathbb{N}_{\mathcal{R}}^t$ , each simple  $r$ -path has length at most  $\ell$ .*

The following statement combines several steps established by Gogacz *et al.* [2018].

**Theorem 5.** *Let  $\psi$  be a UCQ. Let  $\ell, n \in \mathbb{N}$  and let  $\mathcal{I}, \mathcal{I}'$ , and  $\mathcal{J}$  be interpretations such that*

1.  $\mathcal{I} \setminus \Delta^{\mathcal{M}}$  is  $\ell$ -bounded and has bounded degree;
2.  $\mathcal{I}'$  is an  $n$ -proper coloring of  $\mathcal{I}$  with finitely many colors;
3.  $\Delta^{\mathcal{J}} \subseteq \Delta^{\mathcal{I}}$ ,  $A^{\mathcal{J}} = A^{\mathcal{I}} \cap \Delta^{\mathcal{J}}$  for all  $A \in \mathbb{N}_{\mathcal{C}}$ , and for all  $(d, e) \in r^{\mathcal{J}} \setminus r^{\mathcal{I}}$  with  $r \in \mathbb{N}_{\mathcal{R}}$ , there exists  $e'$  such that  $(d, e') \in r^{\mathcal{I}'}$  and  $N_n^{\mathcal{I}'}(e) \simeq N_n^{\mathcal{I}'}(e')$ ;
4.  $\mathcal{J} \setminus \Delta^{\mathcal{M}}$  is  $\ell$ -bounded.

*If  $n$  is large enough with respect to  $\ell, |\psi|$ , and  $|\Delta^{\mathcal{M}}|$ , then  $\mathcal{I}^* \not\models \varphi$  implies  $\mathcal{J}^* \not\models \varphi$ .*

Let us now apply this to our counter-witness  $\mathcal{I}$  with a strongly canonical tree decomposition  $\mathfrak{S}$  of bounded width and outdegree.

The first condition in Theorem 5 is ensured by the properties of  $\mathfrak{S}$ . Indeed, for each element  $d$  outside of  $\Delta^{\mathcal{M}}$ , the degree is bounded by the sum of the sizes of the bags containing  $d$ . But by strong canonicity each such  $d$  occurs only in the bag where it is fresh, and a subset of its children. Because  $\mathfrak{S}$  has bounded degree and width, it follows that the degree of each such  $d$  is also bounded. For  $\ell$ -boundedness it suffices to notice that after removing  $\Delta^{\mathcal{M}}$ , all bags corresponding to a transitive role name  $r$  are disjoint. Consequently, for  $\ell$  we can take any number bounding the size of bags in  $\mathfrak{S}$ .

By Lemma 6, for any  $n$  there exists an  $n$ -proper coloring  $\mathcal{I}'$  of  $\mathcal{I}$  with finitely many colors. We construct  $\mathcal{J}$  from  $\mathcal{I}'$  like before, but for  $v$  and  $u$  we additionally require that the isomorphism  $h$  witnessing  $\mathcal{J}(v) \simeq \mathcal{J}(u)$  preserves  $n$  neighborhoods in  $\mathcal{I}'$ : for each  $d \in \Delta_v$ ,  $N_n^{\mathcal{I}'}(d) \simeq N_n^{\mathcal{I}'}(h(d))$ . One can find such  $v$  and  $u$  on each path because  $\mathfrak{S}$  has bounded width and the size of neighborhoods of radius  $n$  is bounded as well; the latter holds because  $\mathcal{I} \setminus \Delta^{\mathcal{M}}$  has bounded degree. This additional requirement ensures the third condition in Theorem 5.

We claim that the length of the longest simple  $r$ -path avoiding  $\Delta^{\mathcal{M}}$  for any transitive role name  $r$  can only increase by one. Indeed, let us examine what happens when we redirect  $r$ -edges from  $d_v$  with  $\tau(v) = r$ . As  $d_v \notin \Delta^{\mathcal{M}}$ , by the strong canonicity of  $\mathfrak{S}$  we know that  $v$  is the only bag storing  $r$ -edges that contains  $d_v$ . Consequently, all  $r$ -edges that enter  $d_v$  in  $\mathcal{I}$  originate in  $\Delta_v$ . Previous steps of the procedure might have redirected some  $r$ -edges to  $d_v$ , but all these edges originate in elements from the subtree of  $\mathfrak{S}$  rooted at  $v$ , and these elements do not belong to  $\Delta^{\mathcal{M}}$ . Hence, when  $v$  is processed, all these edges disappear, because their origins are removed. Because we only redirect  $r$ -edges to bags that have not been replaced by a single element before, no  $r$ -edge will ever be redirected to  $d_v$ . Thus, we have a global property that each  $r$ -edge in  $\mathcal{J}$  that is a result of a redirection originates in an element that has no incoming  $r$ -edges. This completes the proof of the claim. Let us take for  $\ell$  in Theorem 5 the maximal size of a bag in  $\mathfrak{S}$  plus 1.

Finally, rewriting our PEQ  $\varphi$  as a UCQ  $\psi$ , we can conclude that if  $n$  is sufficiently large,  $\mathcal{J}^* \not\models \varphi$ .

## E Missing proofs for Section 6

We formulate our result slightly stronger in terms of concept satisfiability, which is the problem of deciding, given  $C, \mathcal{T}$ , whether there is a model  $\mathcal{I}$  of  $\mathcal{T}$  with  $C^{\mathcal{I}} \neq \emptyset$ .

**Lemma 7.** *Both finite and unrestricted concept satisfiability relative to  $SIQ^-$  TBoxes over one transitive role are 2EXPTIME-hard.*

*Proof.* We reduce the word problem for exponentially space bounded alternating Turing machines (ATMs). We actually use a slightly unusual ATM model which is easily seen to be equivalent to the standard model.

An *alternating Turing machine (ATM)* is a tuple  $M = (Q, \Theta, \Gamma, q_0, \Delta)$  where  $Q = Q_{\exists} \uplus Q_{\forall}$  is the set of states

that consists of *existential states* in  $Q_{\exists}$  and *universal states* in  $Q_{\forall}$ . Further,  $\Theta$  is the input alphabet and  $\Gamma$  is the tape alphabet that contains a *blank symbol*  $\square \notin \Theta$ ,  $q_0 \in Q_{\exists}$  is the *starting state*, and the *transition relation*  $\Delta$  is of the form  $\Delta \subseteq Q \times \Gamma \times Q \times \Gamma \times \{L, R\}$ . The set  $\Delta(q, \sigma) := \{(q', \sigma', M) \mid (q, \sigma, q', \sigma', M) \in \Delta\}$  must contain exactly two elements for every  $q \in Q$  and  $\sigma \in \Gamma$ . Moreover, the state  $q'$  must be from  $Q_{\forall}$  if  $q \in Q_{\exists}$  and from  $Q_{\exists}$  otherwise, that is, existential and universal states alternate. Thus, for every configuration, there are precisely two successor configurations; we refer to them using the *first* and *second* successor configurations by fixing an (arbitrary) order on  $\Delta(q, \sigma)$ . Note that there is no accepting state. The ATM accepts if it runs forever and rejects otherwise. Starting from the standard ATM model, this can be achieved by assuming that exponentially space bounded ATMs terminate on any input and then modifying them to enter an infinite loop from the accepting state.

A *configuration* of an ATM is a word  $wqw'$  with  $w, w' \in \Gamma^*$  and  $q \in Q$ . We say that  $wqw'$  is *existential* if  $q$  is, and likewise for *universal*. *Successor configurations* are defined in the usual way. Note that every configuration has exactly two successor configurations. We call these the *left* and *right* successor configurations.

A *computation tree* of an ATM  $M$  on input  $w$  is an infinite tree without leaves whose nodes are labeled with configurations of  $M$  such that

- the root is labeled with the initial configuration  $q_0w$ ;
- if an inner node is labeled with an existential configuration  $wqw'$ , then it has a single successor and this successor is labeled with a successor configuration of  $wqw'$ ;
- if an inner node is labeled with a universal configuration  $wqw'$ , then it has two successors and these successors are labeled with the two successor configurations of  $wqw'$ .

An ATM  $M$  *accepts* an input  $w$  if there is a computation tree of  $M$  on  $w$ .

There is a fixed  $2^n$  space bounded ATM  $M$  whose word problem is 2EXPTIME-hard [Chandra *et al.*, 1981]. We assume that  $M$  has been modified so that it never attempts to move left on the left-most tape cell and so that we are only interested in non-empty inputs  $w$ .

Given  $M$  and  $w$ , we construct a TBox  $\mathcal{T}_{M,w}$  using a concept name  $I$  and a single transitive role  $r$  such that  $M$  accepts  $w$  iff  $I$  is satisfiable relative to  $\mathcal{T}_{M,w}$ .

We refrain from repeating the concept inclusions given in the main part, and rather address Points (i) and (iii), and provide the missing details for Point (ii).

For Point (i), we first ensure that there is exactly one leaf labeled with a symbol of shape  $(q, a)$ , by using a fresh concept name  $\text{Head}$  and including the following CIs:

$$\begin{aligned} L_0 &\sqsubseteq (\leq (2^n - 2) r \left( \bigsqcup_{i=1}^n L_i \right)) \\ L_0 &\sqsubseteq (= 1 r (L_n \sqcap \text{Head})) \\ L_n \sqcap \text{Head} &\sqsubseteq \bigsqcup_{(q,a) \in \Sigma} C_{(q,a)}^h \end{aligned}$$

$$L_n \sqcap \neg \text{Head} \sqsubseteq \prod_{(q,a) \in \Sigma} \neg C_{(q,a)}^h$$

Intuitively, the first CI restricts the number of nodes in the tree, so that the enforced tree is *exactly* the expected full binary tree. The second CI states that there is *exactly* one leaf satisfying Head. The remaining CIs enforce that the leaf satisfying Head indeed satisfies some  $C_{(q,a)}^h$ , and that the others do not satisfy such a concept.

It remains to synchronize neighboring leaves according their labeling with symbols  $C_\sigma^x$ . For doing so, we need to make precise how numbers are associated to leaves. A leaf node  $d$  has value  $i \in \{0, \dots, 2^n - 1\}$  precisely if, for all  $j$  with  $1 \leq j \leq n$ , the  $j$ -th bit in the binary encoding of  $i$  is 1 iff  $d$  satisfies  $X_j$ . As a convention, we assume that  $X_0$  is responsible for the least significant bit. It will be convenient to use the abbreviations  $X_i^*$  and  $X_i^+$ ,  $0 \leq i \leq n - 1$ , for

$$\neg X_i \sqcap \prod_{0 \leq k \leq i-1} X_k \quad \text{and} \quad X_i \sqcap \prod_{0 \leq k \leq i-1} \neg X_k,$$

respectively. To synchronize leaves with consecutive numbers, we enforce additional  $r$ -successors as follows. We introduce another set of concept names:  $H$  and  $D_\sigma, D'_\sigma$ , for every  $\sigma \in \Sigma$ . The idea is to introduce for a leaf with value  $i$  and labeling  $C_{\sigma_l}^l, C_{\sigma_h}^h, C_{\sigma_r}^r$  two  $r$ -successors: one with value  $i + 1$  satisfying  $D_{\sigma_n}$  and  $D'_{\sigma_r}$ , and one with value  $i$  satisfying  $D_{\sigma_l}$  and  $D'_{\sigma_h}$ . We additionally require that all these successors satisfy  $H$ . This is realized using the following CIs, for every  $\sigma, \sigma' \in \Sigma$ , every  $i$  with  $0 \leq i < n$ , and every  $j > i$ :

$$\begin{aligned} L_n \sqcap X_i^* \sqcap C_\sigma^h \sqcap C_{\sigma'}^r &\sqsubseteq \exists r. (H \sqcap X_i^+ \sqcap D_\sigma \sqcap D'_{\sigma'}) \\ L_n \sqcap X_i^* \sqcap C_{\sigma_l}^l \sqcap C_{\sigma_h}^h &\sqsubseteq \exists r. (H \sqcap X_i^* \sqcap D_\sigma \sqcap D'_{\sigma'}) \\ L_n \sqcap X_i^* \sqcap X_j &\sqsubseteq \forall r. (H \rightarrow X_j) \\ L_n \sqcap X_i^* \sqcap \neg X_j &\sqsubseteq \forall r. (H \rightarrow \neg X_j) \\ D_\sigma &\sqsubseteq \neg D_{\sigma'} \quad \text{if } \sigma \neq \sigma' \\ D'_\sigma &\sqsubseteq \neg D'_{\sigma'} \quad \text{if } \sigma \neq \sigma' \end{aligned}$$

Now, to enforce the synchronization, we add the concept inclusion

$$L_0 \sqsubseteq (\leq (2^n - 2) r H),$$

forcing some of the newly created successors to identify, which is only possible if they have the same number and the same labeling with the  $D_\sigma, D'_\sigma$ . Using the provided intuitions it is not difficult to verify that:

*Claim 1.* If  $\mathcal{I}$  is a model of the TBox constructed so far,  $d \in L_0^{\mathcal{I}}$ , and  $d_0, \dots, d_{2^n-1}$  are leaf elements reachable from  $d$ , then  $d_0, \dots, d_{2^n-1}$  represent a valid configuration of  $M$ .

For Point (ii), that is, synchronization of successor configurations, we create at the leaves of every enforced tree successors which contain the current configuration and the successor configuration(s) as described in the body of the paper. Using at-most restrictions enforced in elements satisfying  $B_\exists, B_{\forall,1}, B_{\forall,2}$ , we force corresponding successors to join and thus to synchronize. We use additional concept names  $E, S_\exists, S_{\forall}^1, S_{\forall}^2$ . Notice that we need different versions of the concept  $S$  mentioned in the body of the paper, to synchronize

between different parts of the computation, and moreover that  $E$  is used to make a non-deterministic choice for existential configurations. We include the following concept inclusions, for all  $i \in \{1, 2\}$ , and all  $\sigma_l, \sigma_h, \sigma_r \in \Sigma$  which can occur in neighboring cells in a valid configuration of  $M$ :

$$\begin{aligned} L_0 &\sqsubseteq \forall r. E \sqcup \forall r. \neg E \\ L_n \sqcap \exists r^- . A_\exists^i \sqcap \langle \sigma_l, \sigma_h, \sigma_r \rangle \sqcap \neg E &\sqsubseteq \exists r. (S_\exists \sqcap D_{\langle \sigma_l, \sigma_h, \sigma_r \rangle}^1) \\ L_n \sqcap \exists r^- . A_\exists^i \sqcap \langle \sigma_l, \sigma_h, \sigma_r \rangle \sqcap E &\sqsubseteq \exists r. (S_\exists \sqcap D_{\langle \sigma_l, \sigma_h, \sigma_r \rangle}^2) \\ L_n \sqcap \exists r^- . A_{\forall} \sqcap \langle \sigma_l, \sigma_h, \sigma_r \rangle &\sqsubseteq \exists r. (S_{\forall}^1 \sqcap D_{\langle \sigma_l, \sigma_h, \sigma_r \rangle}^1) \\ L_n \sqcap \exists r^- . A_{\forall} \sqcap \langle \sigma_l, \sigma_h, \sigma_r \rangle &\sqsubseteq \exists r. (S_{\forall}^2 \sqcap D_{\langle \sigma_l, \sigma_h, \sigma_r \rangle}^2) \\ L_n \sqcap \exists r^- . A_\exists^i \sqcap C_{\sigma_h}^h &\sqsubseteq \exists r. (S_{\forall}^i \sqcap D_{\sigma_h}) \\ L_n \sqcap \exists r^- . A_{\forall} \sqcap C_{\sigma_h}^h &\sqsubseteq \exists r. (S_\exists \sqcap D_{\sigma_h}) \\ S_{\forall}^i &\sqsubseteq \neg S_{\forall}^{3-i} \\ S_{\forall}^i &\sqsubseteq \neg S_\exists \end{aligned}$$

where  $\langle \sigma_l, \sigma_h, \sigma_r \rangle$  is an abbreviation for  $C_{\sigma_l}^l \sqcap C_{\sigma_h}^h \sqcap C_{\sigma_r}^r$ , and  $D_{\langle \sigma_l, \sigma_h, \sigma_r \rangle}^j$ ,  $j \in \{1, 2\}$  is  $D_\sigma$  if, when in a configuration with neighboring cells  $\sigma_l, \sigma_h, \sigma_r$ , the next label of the current cell in the  $j$ -th successor configuration is  $\sigma$  (recall that every configuration has exactly two successor configurations).

Similar to the what was done before, we propagate the values associated to the leaves to the newly created successors. This is done using the following CIs, for every  $i$  with  $0 \leq i \leq n - 1$  and  $S \in \{S_\exists, S_{\forall}^1, S_{\forall}^2\}$ :

$$\begin{aligned} L_n \sqcap X_j &\sqsubseteq \forall r. (S \rightarrow X_j) \\ L_n \sqcap \neg X_j &\sqsubseteq \forall r. (S \rightarrow \neg X_j) \end{aligned}$$

It remains to give the promised at-most restrictions, for all  $i \in \{1, 2\}$ :

$$B_\exists \sqsubseteq (\leq 2^n r S_\exists), \quad B_{\forall}^i \sqsubseteq (\leq 2^n r S_{\forall}^i).$$

Again, based on the provided intuitions it is not difficult to verify that neighboring configurations are indeed successor configurations according to  $M$ 's transition relation. More precisely, we have:

*Claim 2.* If  $\mathcal{I}$  is a model of the TBox constructed so far, then for all  $d, e, e' \in \Delta^{\mathcal{I}}$  such that  $(d, e), (d, e') \in r^{\mathcal{I}}$  we have:

1. if  $d \in B_\exists^{\mathcal{I}}, e \in (A_\exists^i)^{\mathcal{I}}$  for some  $i \in \{1, 2\}$ , and  $e' \in A_{\forall}^{\mathcal{I}}$ , then the configuration below  $e'$  is the first successor configuration of the configuration below  $e$  if  $e' \in (\forall r. E)^{\mathcal{I}}$ ; and the second successor configuration of the configuration below  $e$  if  $e' \in (\forall r. \neg E)^{\mathcal{I}}$ ;
2. if, for some  $i \in \{1, 2\}$ ,  $d \in (B_{\forall}^i)^{\mathcal{I}}, e \in A_{\forall}^{\mathcal{I}}$ , and  $e' \in (A_\exists^i)^{\mathcal{I}}$ , then the configuration below  $e'$  is the  $i$ -th successor configuration of the configuration below  $e$ .

For Point (iii), that is, the enforcement of the initial configuration, let  $w = a_0 \cdot \dots \cdot a_{n-1}$  be the input word. It is routine to give (polynomially sized) concepts  $(X = k)$ , for  $0 \leq k \leq n - 1$ , describing all leaves with value  $k$ , and  $(X \geq n)$  describing all nodes with value  $\geq n$ . We include the following concept inclusions, for all  $i$  with  $0 < i < n$ :

$$L_n \sqcap \exists r^- . I \sqcap (X = 0) \sqsubseteq C_{(q_0, a_0)}^h$$

$$\begin{aligned} L_n \sqcap \exists r^-. I \sqcap (X = i) &\sqsubseteq C_{a_i}^h \\ L_n \sqcap \exists r^-. I \sqcap (X \geq n) &\sqsubseteq C_{\square}^h. \end{aligned}$$

Recall that  $\square$  is the blank symbol in the tape alphabet. It is not difficult to see that the configuration encoded in the tree starting from  $I$  is the initial configuration.

This finishes the construction of the TBox. Correctness of the reduction is established in the following.

*Claim 3.*  $M$  accepts  $w$  iff  $I$  is satisfiable relative to  $\mathcal{T}_{M,w}$ .

*Proof of Claim 3.* ( $\Rightarrow$ ) If  $M$  accepts  $w$ , there is an infinite alternating computation of  $M$  on input  $w$ . We inductively convert the computation into an interpretation  $\mathcal{I}$  in the expected way:

- Start with a tree whose leaves are labeled with the initial configuration, and whose root is labeled with  $I, A_{\exists}^1, L_0$ .
- Choose some node  $d$  in the interpretation constructed so far satisfying either  $A_{\forall}$  or  $A_{\exists}^i$  and let  $\alpha$  be the configuration the leaves of the tree below  $d$ .
  - if  $d$  satisfies  $A_{\forall}$ , we inductively know that  $\alpha$  is a universal configuration and has two successor configurations  $\alpha_1, \alpha_2$  in the accepting computation. We add new elements  $e_1, e_2, f_1, f_2$  to  $\mathcal{I}$  such that, for  $i \in \{1, 2\}$ ,  $e_i \in (B_{\forall}^i)^{\mathcal{I}}, f_i \in (A_{\exists}^i \sqcap L_0)^{\mathcal{I}}$ , and  $(e_i, d) \in r^{\mathcal{I}}$ , and  $(e_i, f_i) \in r^{\mathcal{I}}$ . Moreover, add below  $e_i$  a tree with configuration  $\alpha_i$  in the leaves.
  - if  $d$  satisfies  $A_{\exists}^i$ , we inductively know that  $\alpha$  is an existential configuration and has one successor configurations  $\alpha'$  in the accepting computation. If  $\alpha'$  is the second successor of  $\alpha$  (according to  $\Delta$ ), we add all elements in the tree below  $d$  to  $E^{\mathcal{I}}$ . Additionally, add new elements  $e, f$  to  $\mathcal{I}$  such that  $e \in B_{\exists}^{\mathcal{I}}, f \in (A_{\forall} \sqcap L_0)^{\mathcal{I}}$ , and  $(e, d) \in r^{\mathcal{I}}$ , and  $(e, f) \in r^{\mathcal{I}}$ . Moreover, add below  $e$  a tree with configuration  $\alpha'$  in the leaves.

It is routine to verify that the interpretation  $\mathcal{I}$  obtained in the limit is a model of  $I$  and  $\mathcal{T}_{M,w}$ .

( $\Leftarrow$ ) Let  $\mathcal{I}$  be a model of  $\mathcal{T}_{M,w}$  and  $d_0 \in I^{\mathcal{I}}$ . By construction of  $\mathcal{T}_{M,w}$  (in particular, the concept inclusions starting with  $I$  from the body of the paper), there is an infinite tree  $(T, \tau)$  labeled with elements from  $\Delta^{\mathcal{I}}$  and having the following properties:

- the root node is labeled with  $d_0$ , that is,  $\tau(\varepsilon) = d_0$ ;
- $T$  has outdegree one in odd levels (assuming  $d$  is in the first level) and outdegree two in even levels;
- nodes  $n$  in odd levels of  $T$  satisfy  $\tau(n) \in (A_{\exists}^i \sqcap L_0)^{\mathcal{I}}$ , for some  $i \in \{1, 2\}$ , and have a single successor  $n'$  such that there is some  $e \in \Delta^{\mathcal{I}}$  with  $e \in B_{\exists}^{\mathcal{I}}$  and  $(e, \tau(n)), (\tau(n'), e) \in r^{\mathcal{I}}$ ;
- nodes  $n$  in even levels of  $T$  satisfy  $\tau(n) \in (A_{\forall} \sqcap L_0)^{\mathcal{I}}$  and have two successors  $n_1, n_2$  such that there are  $e_1, e_2 \in \Delta^{\mathcal{I}}$  with  $e_i \in (B_{\forall}^i)^{\mathcal{I}}, (e_i, \tau(n)), (\tau(n'), e_i) \in r^{\mathcal{I}}$ , and  $\tau(n_i) \in (A_{\exists}^i)^{\mathcal{I}}$ ;

Note that  $T$  has the structure of an infinite alternating computation of  $M$ . It remains to associate a configuration to every

node in the tree. By construction of  $T$ , we have  $\tau(n) \in L_0^{\mathcal{I}}$ , for all nodes  $n \in T$ . By Claim 1, there is a tree labeled with a configuration below each  $\tau(n)$ .

By Point (iii), we know that the configuration in the below  $d_0$  is the initial configuration  $\alpha_0$  of  $M$  on input  $w$ . We can now use Claim 2 and the construction of  $T$  to inductively construct an infinite, alternating computation of  $M$  on input  $w$ . Thus  $M$  accepts  $w$ .

This finishes the proof of the claim, and in fact of 2EXPTIME-hardness in the unrestricted case. For finite reasoning, we have to show that  $I$  is satisfiable relative to  $\mathcal{T}_{M,w}$  iff it is finitely satisfiable relative to  $\mathcal{T}_{M,w}$ . Since the “if”-direction is trivial, we focus on the “only if”-direction.

It suffices to show that there is a finite model  $\mathcal{I}$  of  $I$  and  $\mathcal{T}_{M,w}$  in case  $M$  accepts  $w$ . We can vary the construction in the ( $\Rightarrow$ )-direction of the proof of Claim 3 as follows. Instead of adding new elements in every step of the inductive construction, we can reuse old elements in case the new element is associated to the same configuration as the old one. Since  $M$  is space bounded, this will happen on every possible path, and hence we end up with a finite model.  $\square$