Consequence-Driven Reasoning for Horn $\mathcal{SHIQ}$ Ontologies

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Abstract

We present a novel reasoning procedure for Horn $\mathcal{SHIQ}$ ontologies—$\mathcal{SHIQ}$ ontologies that can be translated to the Horn fragment of first-order logic. In contrast to traditional reasoning procedures for ontologies, our procedure does not build models or model representations, but works by deriving new consequent axioms. The procedure is closely related to the so-called completion-based procedure for $\mathcal{EL}^{++}$ ontologies, and can be regarded as an extension thereof. In fact, our procedure is theoretically optimal for Horn $\mathcal{SHIQ}$ ontologies as well as for the common fragment of $\mathcal{EL}^{++}$ and $\mathcal{SHIQ}$.

A preliminary empirical evaluation of our procedure on large medical ontologies demonstrates a dramatic improvement over existing ontology reasoners. Specifically, our implementation allows the classification of the largest available OWL version of Galen. To the best of our knowledge no other reasoner is able to classify this ontology.

1 Introduction

Ontologies are formal vocabularies of terms describing specific subjects like chemical elements, genes, or animal species. The terms in ontologies are "defined" by means of relationships with other terms of the ontology using *ontology languages*. Ontology languages based on Description Logics (DLs) [Baader *et al.*, 2007], such as OWL,[1] are becoming increasingly popular among ontology developers thanks to the availability of *ontology reasoners*, which provide automated support for visualization, debugging, and querying of ontologies. *Classification* is a central reasoning service provided by ontology reasoners. The goal of classification is to compute a hierarchical relation between classes. The class hierarchy is used to browse ontologies in ontology editors.

Most of the currently-available ontology reasoners are based on so-called *model building procedures* such as tableau [Horrocks *et al.*, 2000] and hyper-tableau [Motik *et al.*, 2007] calculi. Such procedures classify an input ontology, in general, by iterating over all necessary pairs of classes, and trying to build a model of the ontology that violates the subsumption relation between them. Recent investigations of tractable DLs such as $\mathcal{EL}^{++}$ [Baader *et al.*, 2005] led to the discovery of another type of reasoning procedures. Instead of enumerating pairs of classes and building counter-models, the procedure for $\mathcal{EL}^{++}$ derives subsumption relations explicitly using special inference rules. The advantage of this method is that subsumption relations are computed "all at once" in a goal-directed way without costly enumerations.

The $\mathcal{EL}^{++}$ language sacrifices many commonly-used constructors, such as inverse roles and functional restrictions, in order to ensure that reasoning is tractable. In this paper we describe a reasoning procedure, which utilizes the core reasoning technique of $\mathcal{EL}^{++}$, but works for a larger class of so-called Horn $\mathcal{SHIQ}$ ontologies. Horn $\mathcal{SHIQ}$ ontologies are ontologies expressed in the DL $\mathcal{SHIQ}$, which do not contain "non-deterministic" constructors, such as positive disjunction: $A \sqsubseteq B \sqcup C$. Horn $\mathcal{SHIQ}$ originally has drawn attention in [Hustadt *et al.*, 2007] due to its tractable *data complexity*. Our paper demonstrates that Horn $\mathcal{SHIQ}$ ontologies also admit for a more efficient classification procedure.

This paper is organised as follows. In the preliminaries we introduce Horn $\mathcal{SHIQ}$ and a completion-based procedure for a fragment of $\mathcal{EL}^{++}$. In Section 3 we discuss how to extend this procedure for new constructors in Horn $\mathcal{SHIQ}$. In Section 4 we present our reasoning procedure and prove soundness, completeness, and termination. Finally, in Section 5 we present an empirical comparison of a prototypical implementation of our procedure with other reasoners, which demonstrates a substantial performance improvement.

2 Preliminaries

In this section we define the description logics $\mathcal{SHIQ}$ and $\mathcal{EL}^{+}$, as well as their fragments Horn $\mathcal{SHIQ}$ and $\mathcal{ELH}$. To simplify the presentation and save space, we will not consider ABox assertions in this paper.

2.1 The Description Logic $\mathcal{SHIQ}$

A description logic *vocabulary* consists of countably infinite sets N_C of *atomic concepts*, and N_R of *atomic roles*. A $\mathcal{SHIQ}$ *role* is either $r \in \mathsf{N}_R$ or an *inverse role* r^- with $r \in \mathsf{N}_R$. We denote by R^- the *inverse of a role* R defined by $R^- := r^-$ when $R = r$ and $R^- := r$ when $R = r^-$.

The syntax and semantics of $\mathcal{SHIQ}$ is summarized in Table 1. The set of $\mathcal{SHIQ}$ *concepts* is recursively defined using

[1] `http://www.w3.org/2004/OWL/`

Name	Syntax	Semantics
Concepts		
atomic concept	A	$A^{\mathcal{I}}$ (given)
top concept	$\top$	$\Delta^{\mathcal{I}}$
bottom concept	$\bot$	$\emptyset$
negation	$\neg C$	$\Delta^{\mathcal{I}} \setminus C^{\mathcal{I}}$
conjunction	$C \sqcap D$	$C^{\mathcal{I}} \cap D^{\mathcal{I}}$
disjunction	$C \sqcup D$	$C^{\mathcal{I}} \cup D^{\mathcal{I}}$
existential restriction	$\exists R.C$	$\{x \mid R^{\mathcal{I}}(x, C^{\mathcal{I}}) \neq \emptyset\}$
universal restriction	$\forall R.C$	$\{x \mid R^{\mathcal{I}}(x, \Delta^{\mathcal{I}} \setminus C^{\mathcal{I}}) = \emptyset\}$
min cardinality	$\geqslant nS.C$	$\{x \mid \|S^{\mathcal{I}}(x, C^{\mathcal{I}})\| \geq n\}$
max cardinality	$\leqslant mS.C$	$\{x \mid \|S^{\mathcal{I}}(x, C^{\mathcal{I}})\| \leq m\}$
Axioms		
role inclusion	$R_1 \sqsubseteq R_2$	$R_1^{\mathcal{I}} \subseteq R_2^{\mathcal{I}}$
role transitivity	$\mathsf{Tra}(R)$	$R^{\mathcal{I}} \circ R^{\mathcal{I}} \subseteq R^{\mathcal{I}}$
concept inclusion	$C \sqsubseteq D$	$C^{\mathcal{I}} \subseteq D^{\mathcal{I}}$

Table 1: The syntax and semantics of $\mathcal{SHIQ}$ terminologies

the constructors given in the upper part of Table 1, where $A \in \mathsf{N}_C$, C, D are concepts, R, S roles, and n, m positive integers. A *terminology* or *ontology* is a set $\mathcal{O}$ of axioms specified in the lower part of Table 1. A role R is *transitive (in $\mathcal{O}$)* if $\mathsf{Tra}(R) \in \mathcal{O}$ or $\mathsf{Tra}(R^-) \in \mathcal{O}$. Given an ontology $\mathcal{O}$, let $R_1 \sqsubseteq_{\mathcal{O}} R_2$ be the smallest transitive reflexive relation between roles such that $R_1 \sqsubseteq R_2 \in \mathcal{O}$ implies $R_1 \sqsubseteq_{\mathcal{O}} R_2$ and $R_1^- \sqsubseteq_{\mathcal{O}} R_2^-$. It is required that for every concept of the form $\geqslant nS.C$ and $\leqslant mS.C$ in $\mathcal{O}$ the role S is *simple*, that is, $R \sqsubseteq_{\mathcal{O}} S$ holds for no transitive role R.

The semantics of $\mathcal{SHIQ}$ is defined using interpretations. An *interpretation* is a pair $\mathcal{I} = (\Delta^{\mathcal{I}}, \cdot^{\mathcal{I}})$ where $\Delta^{\mathcal{I}}$ is a non-empty set called *the domain of the interpretation* and $\cdot^{\mathcal{I}}$ is the *interpretation function*, which assigns to every $A \in \mathsf{N}_C$ a set $A^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}}$, and to every $r \in \mathsf{N}_R$ a relation $r^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}} \times \Delta^{\mathcal{I}}$. The interpretation is extended to roles by $(r^-)^{\mathcal{I}} := \{\langle x, y\rangle \mid \langle y, x\rangle \in r^{\mathcal{I}}\}$ and to concepts according to the right column of Table 1, where $\rho(x, U)$ for $\rho \in \Delta^{\mathcal{I}} \times \Delta^{\mathcal{I}}$, $U \subseteq \Delta^{\mathcal{I}}$, and $x \in \Delta^{\mathcal{I}}$ denotes the set $\{y \mid \langle x, y\rangle \in \rho \wedge y \in U\}$, and $\|V\|$ denotes the cardinality of a set $V \subseteq \Delta^{\mathcal{I}}$. An interpretation $\mathcal{I}$ *satisfies an axiom* α (written $\mathcal{I} \models \alpha$) if the respective condition to the right of the axiom in Table 1 holds; $\mathcal{I}$ is a *model of an ontology* $\mathcal{O}$ (written $\mathcal{I} \models \mathcal{O}$) if $\mathcal{I}$ satisfies every axiom in $\mathcal{O}$. We say that α is a *(logical) consequence* of $\mathcal{O}$, or *is entailed* by $\mathcal{O}$ (written $\mathcal{O} \models \alpha$) if every model of $\mathcal{O}$ satisfies α.

Classification is a key reasoning problem for description logics and ontologies, which requires to compute all *subsumptions* $A \sqsubseteq B$ entailed by $\mathcal{O}$ between atomic concepts.

2.2 The Horn Fragment of $\mathcal{SHIQ}$

Positive and *negative polarities* of occurrences of $\mathcal{SHIQ}$ concepts in concepts and axioms are defined as follows:

- C occurs positively in C;
- C occurs positively (negatively) in $\neg C_-$, $C_+ \sqcap D_+$, $C_+ \sqcup D_+$, $\exists R.C_+$, $\forall R.C_+$, $\geqslant nS.C_+$, $\leqslant mS.C_-$, and $C_- \sqsubseteq D_+$ if C occurs positively (negatively) in C_+ or in D_+, or negatively (positively) in C_- (when applicable).

A concept C occurs *positively* (*negatively*) in an ontology $\mathcal{O}$ if C occurs positively (negatively) in some axiom of $\mathcal{O}$. Note that it is possible for a concept to occur positively and negatively at the same time in an axiom or an ontology.

A $\mathcal{SHIQ}$ ontology $\mathcal{O}$ is *Horn* if:

- no concept of the form $C \sqcup D$ or $\leqslant mR.C$ with $m > 1$ occurs positively in $\mathcal{O}$;
- no concept of the form $\neg C$, $\forall R.C$, $\geqslant nR.C$ with $n > 1$, or $\leqslant mR.C$ occurs negatively in $\mathcal{O}$.

2.3 Structural Transformation

Structural transformation is used to simplify the axioms of the ontology preserving its "structure". Given a $\mathcal{SHIQ}$ ontology $\mathcal{O}$, for every (sub-)concept C in $\mathcal{O}$ we introduce a fresh atomic concept A_C and define a function $\mathsf{st}(C)$ by:

- $\mathsf{st}(A) = A$, $\mathsf{st}(\top) = \top$, $\mathsf{st}(\bot) = \bot$;
- $\mathsf{st}(\neg C) = \neg A_C$;
- $\mathsf{st}(C \sqcap D) = A_C \sqcap A_D$; $\mathsf{st}(C \sqcup D) = A_C \sqcup A_D$
- $\mathsf{st}(\exists R.C) = \exists R.A_C$; $\mathsf{st}(\forall R.C) = \forall R.A_C$;
- $\mathsf{st}(\geqslant nR.C) = \geqslant nR.A_C$; $\mathsf{st}(\leqslant mR.C) = \leqslant mR.A_C$.

The result of applying *structural transformation* to $\mathcal{O}$ is an ontology $\mathcal{O}'$ that contains all role inclusion and role transitivity axioms in $\mathcal{O}$ in addition to the following axioms:

- $A_C \sqsubseteq \mathsf{st}(C)$ for every C occurring positively in $\mathcal{O}$
- $\mathsf{st}(C) \sqsubseteq A_C$ for every C occurring negatively in $\mathcal{O}$
- $A_C \sqsubseteq A_D$ for every concept inclusion $C \sqsubseteq D \in \mathcal{O}$

It can be shown that structural transformation preserves the logical consequences of ontological axioms.

Proposition 1 *Let $\mathcal{O}'$ be obtained from $\mathcal{O}$ by structural transformation. Then for every axiom α containing no introduced atomic concepts A_C, we have $\mathcal{O} \models \alpha$ iff $\mathcal{O}' \models \alpha$.*

2.4 The Description Logic $\mathcal{EL}^+$

The description logic $\mathcal{EL}^+$ is one of the few description logics for which standard reasoning problems are decidable in polynomial time. $\mathcal{EL}^+$ allows only for concepts constructed from atomic concepts A and the top concept $\top$ using conjunction $C \sqcap D$ and existential restriction $\exists r.C$, where r is an atomic role. The axioms of $\mathcal{EL}^+$ can be either concept inclusions $C \sqsubseteq D$ or *complex role inclusions* of the form $r_1 \circ \cdots \circ r_n \sqsubseteq s$. The last are interpreted in $\mathcal{I}$ as $r_1^{\mathcal{I}} \circ \cdots \circ r_n^{\mathcal{I}} \subseteq s^{\mathcal{I}}$, where $\circ$ is a composition of binary relations. For the purpose of this paper, we consider a common fragment of $\mathcal{EL}^+$ and $\mathcal{SHIQ}$ called $\mathcal{ELH}$, which allows only for (simple) role inclusions of the form $r \sqsubseteq s$. It can be easily seen that every $\mathcal{ELH}$ ontology is a Horn $\mathcal{SHIQ}$ ontology since it cannot contain concepts of the form $\neg C$, $C \sqcup D$, $\forall R.C$, $\geqslant nR.C$, or $\leqslant mR.C$.

In [Baader *et al.*, 2005], a polynomial time classification procedure has been presented for the description logic $\mathcal{EL}^{++}$, which extends $\mathcal{EL}^+$ with the bottom concept $\bot$, nominals, and "safe" concrete domains. The procedure uses a number of so-called *completion rules* that derive new concept inclusions. In Table 2 we list the completion rules relevant to $\mathcal{ELH}$. The rules are applied to a *normalised* $\mathcal{ELH}$ ontology $\mathcal{O}$ that is

$$\textbf{IR1}\ \frac{}{A \sqsubseteq A} \qquad \textbf{IR2}\ \frac{}{A \sqsubseteq \top}$$

$$\textbf{CR1}\ \frac{A \sqsubseteq B \quad B \sqsubseteq C \in \mathcal{O}}{A \sqsubseteq C}$$

$$\textbf{CR2}\ \frac{A \sqsubseteq B \quad A \sqsubseteq C \quad B \sqcap C \sqsubseteq D \in \mathcal{O}}{A \sqsubseteq D}$$

$$\textbf{CR3}\ \frac{A \sqsubseteq B \quad B \sqsubseteq \exists r.C \in \mathcal{O}}{A \sqsubseteq \exists r.C}$$

$$\textbf{CR4}\ \frac{A \sqsubseteq \exists r.B \quad r \sqsubseteq s \in \mathcal{O}}{A \sqsubseteq \exists s.B}$$

$$\textbf{CR5}\ \frac{A \sqsubseteq \exists r.B \quad B \sqsubseteq C \quad \exists r.C \sqsubseteq D \in \mathcal{O}}{A \sqsubseteq D}$$

Table 2: The Completion Rules for $\mathcal{ELH}$

obtained from the input ontology by structural transformation and simplification. Structural transformation for $\mathcal{ELH}$ produces only axioms of the form (1) $A \sqsubseteq B$, (2) $A \sqcap B \sqsubseteq C$, (3) $A \sqsubseteq B \sqcap C$, (4) $A \sqsubseteq \exists r.B$, (5) $\exists r.A \sqsubseteq B$, and (6) $r \sqsubseteq s$, where A, B, and C are atomic concepts or $\top$, and r, s atomic roles. Axioms $A \sqsubseteq B \sqcap C$ of form (3) are then replaced with a pair of axioms $A \sqsubseteq B$ and $A \sqsubseteq C$ of form (1).

The completion rules in Table 2 derive new axioms of the form $A \sqsubseteq B$ and $C \sqsubseteq \exists r.D$ from axioms in $\mathcal{O}$ and other axioms of these forms already derived, where A, B, C, and D are atomic concepts or $\top$, and r, s atomic roles.[2] In [Baader *et al.*, 2005] it was shown that the rules **IR1**–**CR5** are *complete for classification*, that is, a concept subsumption $A \sqsubseteq B$ is entailed by $\mathcal{O}$ if and only if it is derivable by these rules.

3 From $\mathcal{ELH}$ to Horn $\mathcal{SHIQ}$

Horn $\mathcal{SHIQ}$ extends $\mathcal{ELH}$ by allowing many new constructors, notably, inverse roles, functionality restrictions, and positive occurrences of universal restrictions. These constructors have been disallowed in $\mathcal{ELH}$ and $\mathcal{EL}^{++}$ for complexity reasons—in [Baader *et al.*, 2005; 2008] it was shown that adding any of these constructors results in a complexity increase from PTime to ExpTime. In this section we give an informal explanation for this complexity increase and outline how the completion-based procedure for $\mathcal{ELH}$ can be extended to handle the new Horn $\mathcal{SHIQ}$ constructors.

3.1 Inverse Roles and Universal Restrictions

According to the definition in Section 2.2, Horn $\mathcal{SHIQ}$ ontologies allow for the usage of inverse roles and positive occurrences of universal restrictions. In fact, positive occurrences of universal restrictions can be expressed by means of inverse roles using the equivalence (1):

$$A \sqsubseteq \forall R.B \qquad \Leftrightarrow \qquad \exists R^-.A \sqsubseteq B \tag{1}$$

[2] In the original presentation [Baader *et al.*, 2005], instead of deriving new axioms $A \sqsubseteq B$ and $C \sqsubseteq \exists r.D$, the completion rules add B to the set $S(A)$ and a pair (C, D) to the set $R(r)$. Thus the set $S(A)$ represents the set of super-concepts of A and the set $R(r)$ represents the pairs of concepts that are existentially related via r.

The increase in the complexity of reasoning with inverse roles and universal restrictions, can be partially explained by a new kind of interaction between these constructors. Axioms of the form $A \sqsubseteq \exists R.B$ and $C \sqsubseteq \forall S.D$ can interact in two ways. First, the following inference (2) is possible:

$$\frac{A \sqsubseteq \exists R.B \qquad B \sqsubseteq \forall R^-.D}{A \sqsubseteq D} \tag{2}$$

It is easy to see using equivalence (1) that (2) is an instance of **CR5** in Table 2. A new kind of interaction is inference (3):

$$\frac{A \sqsubseteq \exists R.B \qquad C \sqsubseteq \forall R.D}{A \sqcap C \sqsubseteq \exists R.(B \sqcap D)} \tag{3}$$

In contrast to (2), and all inference rules in Table 2, which have only conclusions of the form $A \sqsubseteq B$ or $A \sqsubseteq \exists R.B$, repeated applications of (3) can produce axioms of the form $\bigsqcap A_i \sqsubseteq \exists R.\bigsqcap B_j$, where $\bigsqcap A_i$ and $\bigsqcap B_j$ are arbitrary conjunctions of atomic concepts. The number of such axioms is no longer polynomially bounded. Note, however, that there are at most exponentially many (semantically non-equivalent) axioms of this form since the number of different concepts in the conjunctions is always bounded. We will use this property to establish an exponential upper bound for our procedure.

3.2 Functional Restrictions on Roles

Horn $\mathcal{SHIQ}$ allow for expressing a functional restriction for a simple role S using the constructor $\leqslant 1 S.\top$. Since, for a functional role S, the axiom $C \sqsubseteq \exists S.D$ implies $C \sqsubseteq \forall S.D$, the following analogs of inferences (3) and (2) are possible:

$$\frac{A \sqsubseteq \exists S.B \qquad C \sqsubseteq \exists S.D \qquad A \sqsubseteq \leqslant 1 S.\top}{A \sqcap C \sqsubseteq \exists S.(B \sqcap D)} \tag{4}$$

$$\frac{A \sqsubseteq \exists S.B \qquad B \sqsubseteq \exists S^-.C \qquad B \sqsubseteq \leqslant 1 S^-.\top}{A \sqsubseteq C} \tag{5}$$

In Section 4, we generalize inferences (2)–(5) and present a sound and complete system of inference rules for Horn $\mathcal{SHIQ}$ ontologies, which derive only consequence axioms of the form $\bigsqcap A_i \sqsubseteq B$ and $\bigsqcap A_i \sqsubseteq \exists R.(\bigsqcap B_j)$.

4 The Calculus for Horn $\mathcal{SHIQ}$ Ontologies

In this section we present a consequence-based procedure for classifying Horn $\mathcal{SHIQ}$ ontologies. The procedure consists of a *preprocessing stage* that applies structural transformation, simplifications, and elimination of transitivity, and a *saturation stage* that applies inferences to derive new axioms.

4.1 Normalization

From now on we use $A_{(i)}$, $B_{(i)}$ to denote atomic concepts, $R_{(i)}$ roles, and $S_{(i)}$ simple roles. We say that a concept C is *simple* if it is of the form $\bot$, A, $\exists R.A$, $\forall R.A$, or $\leqslant 1 S.A$. We denote by $\bigsqcap A_i$ a (possibly empty) conjunction of atomic concepts. The empty conjunction is abbreviated to $\top$.

Lemma 2 *Every Horn $\mathcal{SHIQ}$ ontology $\mathcal{O}$ can be transformed into an ontology $\mathcal{O}'$ containing only axioms of the forms: (n1) $\bigsqcap A_i \sqsubseteq C$, (n2) $R_1 \sqsubseteq R_2$, and (n3) $\mathsf{Tra}(R)$, where C is a simple concept. The transformation preserves (non)entailment of axioms α over the signature of $\mathcal{O}$ and can be performed in polynomial time assuming unary coding of numbers.*

Proof. By applying structural transformation to $\mathcal{O}$, we obtain an ontology $\mathcal{O}'$ containing only concept inclusions of the form $A_1 \sqsubseteq A_2$, $A \sqsubseteq \mathsf{st}(C_+)$, and $\mathsf{st}(C_-) \sqsubseteq A$, where C_+ occurs positively in $\mathcal{O}$ and C_- occurs negatively in $\mathcal{O}$. Since $\mathcal{O}$ is a Horn $\mathcal{SHIQ}$ ontology, C_+ can only be of the form $\top$, $\bot$, A, $\neg C$, $C \sqcap D$, $\exists R.C$, $\forall R.C$, $\geqslant nS.C$, or $\leqslant 1S.C$, and C_- only of the form $\top$, $\bot$, A, $C \sqcap D$, $C \sqcup D$, $\exists R.C$, or $\geqslant 1R.C$.

Concept inclusions of the form $A \sqsubseteq \mathsf{st}(C_+)$ that are not of form (n1), are transformed to form (n1) as follows:

- $A \sqsubseteq \mathsf{st}(\neg C) = \neg A_C \;\Rightarrow\; A \sqcap A_C \sqsubseteq \bot$;
- $A \sqsubseteq \mathsf{st}(\geqslant nS.C) = \geqslant nS.A_C \;\Rightarrow\; A \sqsubseteq \exists S.B_i$, $B_i \sqsubseteq A_C$, $1 \leq i \leq n$, $B_i \sqcap B_j \sqsubseteq \bot$, $1 \leq i < j \leq n$, where B_i are fresh atomic concepts.

Concept inclusions of the form $\mathsf{st}(C_-) \sqsubseteq A$ that are not of form (n1) are transformed to form (n1) as follows:

- $\mathsf{st}(C \sqcup D) = A_C \sqcup A_D \sqsubseteq A \;\Rightarrow\; A_C \sqsubseteq A, A_D \sqsubseteq A$;
- $\mathsf{st}(\exists R.C) = \exists R.A_C \sqsubseteq A \;\Rightarrow\; A_C \sqsubseteq \forall R^-.A$;
- $\mathsf{st}(\geqslant 1S.C) = \geqslant 1S.A_C \sqsubseteq A \;\Rightarrow\; A_C \sqsubseteq \forall S^-.A$.

It is easy to show using Proposition 1, that $\mathcal{O}' \models \alpha$ iff $\mathcal{O} \models \alpha$ for every axiom α containing no new symbols. ☐

4.2 Elimination of Transitivity

After normalization, we apply a well-known technique, which allows the elimination of transitivity axioms. Transitivity axioms of form (n3) in Lemma 2 can interact only with axioms $\bigsqcap A_i \sqsubseteq \forall R.B$ of form (n2) through role inclusions (n3). The transformation introduces a triple of axioms (6) for every axiom $\bigsqcap A_i \sqsubseteq \forall R.B$ of form (n1) and every transitive sub-role T of R, where B^T is a fresh atomic concept:

$$\bigsqcap A_i \sqsubseteq \forall T.B^T \qquad B^T \sqsubseteq \forall T.B^T \qquad B^T \sqsubseteq B \qquad (6)$$

Intuitively, B^T is used to propagate B to all elements reachable from elements in $\bigsqcap A_i$ via a T-chain.

Lemma 3 *Let $\mathcal{O}$ be consisting of axioms of forms (n1)–(n3) in Lemma 2, and $\mathcal{O}'$ be obtained from $\mathcal{O}$ by adding axioms (6) as described above and removing all transitivity axioms (n3). Then for every axiom α that does not contain concepts B^T and non-simple roles, we have $\mathcal{O} \models \alpha$ iff $\mathcal{O}' \models \alpha$.*

Proof (sketch). It is sufficient to show that (i) every model $\mathcal{I}$ of $\mathcal{O}$ can be turned into a model $\mathcal{J}$ of $\mathcal{O}'$ by (re-)interpreting concepts B^T, and conversely, (ii) every model $\mathcal{J}$ of $\mathcal{O}'$ can be turned into a mode $\mathcal{I}$ of O by (re-)interpreting non-simple roles. Both of these transformations preserve the interpretation of axioms α that do not contain these symbols.

For proving (i), we interpret B^T in $\mathcal{J}$ as $(B \sqcap \forall T.B)^{\mathcal{I}}$. Trivially, the last two axioms in (6) are satisfied in $\mathcal{J}$. The first axiom in (6) is satisfied in $\mathcal{J}$ since $\mathcal{J}$ satisfies $\bigsqcap A_i \sqsubseteq \forall R.B$ and T is a transitive sub-role of R. $\mathcal{J}$ satisfies the remaining axioms in $\mathcal{O}'$ since they do not contain the new concepts B^T.

For proving (ii), we interpret every non-simple role R in $\mathcal{I}$ as the union of $R^{\mathcal{J}}$ and the transitive closures of $T^{\mathcal{J}}$ for every transitive sub-role T of R ($T^{\mathcal{J}}$ is not necessarily a transitive relation since $\mathcal{O}'$ does not contain the transitivity axioms). It is easy to show that $\mathcal{I}$ satisfies all axioms (n1)–(n3). In particular, $\mathcal{I}$ satisfies the axioms of the form $\bigsqcap A_i \sqsubseteq \forall R.B$ since $\mathcal{I}$ remains to be a model of axioms (6). ☐

$$\textsf{I1}\;\frac{}{M \sqcap A \sqsubseteq A} \qquad \textsf{I2}\;\frac{}{M \sqsubseteq \top}$$

$$\textsf{R1}\;\frac{M \sqsubseteq A_i \quad \bigsqcap A_i \sqsubseteq C \in \mathcal{O}}{M \sqsubseteq C}$$

$$\textsf{R2}\;\frac{M \sqsubseteq \exists R.N \quad N \sqsubseteq \bot}{M \sqsubseteq \bot}$$

$$\textsf{R3}\;\frac{M \sqsubseteq \exists R_1.N \quad M \sqsubseteq \forall R_2.A \quad R_1 \sqsubseteq_{\mathcal{O}} R_2}{M \sqsubseteq \exists R_1.(N \sqcap A)}$$

$$\textsf{R4}\;\frac{M \sqsubseteq \exists R_1.N \quad N \sqsubseteq \forall R_2.A \quad R_1 \sqsubseteq_{\mathcal{O}} R_2^-}{M \sqsubseteq A}$$

$$\textsf{R5}\;\frac{\begin{array}{lll} M \sqsubseteq \exists R_1.N_1 & N_1 \sqsubseteq B & R_1 \sqsubseteq_{\mathcal{O}} S \\ M \sqsubseteq \exists R_2.N_2 & N_2 \sqsubseteq B & R_2 \sqsubseteq_{\mathcal{O}} S \\ M \sqsubseteq \leqslant 1S.B & & \end{array}}{M \sqsubseteq \exists R_1.(N_1 \sqcap N_2)}$$

$$\textsf{R6}\;\frac{\begin{array}{lll} M \sqsubseteq \exists R_1.N_1 & N_1 \sqsubseteq \exists R_2.(N_2 \sqcap A) & R_1 \sqsubseteq_{\mathcal{O}} S^- \\ M \sqsubseteq B & N_2 \sqcap A \sqsubseteq B & R_2 \sqsubseteq_{\mathcal{O}} S \\ N_1 \sqsubseteq \leqslant 1S.B & & \end{array}}{M \sqsubseteq A \quad M \sqsubseteq \exists R_2^-.N_1}$$

Table 3: Saturation Rules for Horn $\mathcal{SHIQ}$ Ontologies

4.3 The Inference Rules

Our procedure for Horn $\mathcal{SHIQ}$ ontologies works by saturating the input axioms under the rules in Table 3. The rules are applied to a preprocessed ontology containing axioms of form (n1) and (n2) in Lemma 2, and produce axioms of the form $M \sqsubseteq C$ and $M \sqsubseteq \exists R.N$, where M and N are conjunctions of atomic concepts, and C is a simple concept.

Rules **I1** and **I2** produce the initial (tautological) concept inclusions for arbitrary M and A, which are then extended using axioms in $\mathcal{O}$ by rule **R1**. Rules **R2**–**R6** are specific to the kinds of simple concepts implied by the conjunctions. Rule **R2** propagates the entailment of bottom backwards over existential restrictions. Rules **R3** and **R4** deal with universal restrictions and generalize respectively inferences (3) and (2) in Section 3.1. Likewise, rules **R5** and **R6** with 7 premises, deal with qualified functional restrictions and generalize inferences (4) and (5). Note that in contrast to (5), rule **R6** has two conclusions. Rules **R3**–**R6** assume that the closure $R_1 \sqsubseteq_{\mathcal{O}} R_2$ of role inclusions of form (n2) is computed. The inference rules **I1**–**R6** are applied exhaustively until no new axiom can be derived. The resulting ontology $\mathcal{O}'$ is called *the saturation* of $\mathcal{O}$.

4.4 Soundness and Completeness

In this section we demonstrate that our procedure is sound and complete for classification, that is, it derives all subsumptions between atomic concepts in the input ontology.

Theorem 4 *Let $\mathcal{O}$ be an ontology containing only axioms of the form (n1) and (n2) in Lemma 2 and $\mathcal{O}'$ the saturation of $\mathcal{O}$ under the rules in Table 3. Then (i) $\mathcal{O} \models M \sqsubseteq B$ iff $M \sqsubseteq \bot \in \mathcal{O}'$ or $M \sqsubseteq B \in \mathcal{O}'$, and (ii) $\mathcal{O} \models M \sqsubseteq \exists R.N$*

iff $M \sqsubseteq \bot \in \mathcal{O}'$ *or there exists* $M \sqsubseteq \exists R_1.N_1 \in \mathcal{O}'$ *such that* $R_1 \sqsubseteq_{\mathcal{O}} R$ *and* $N_1 \sqsubseteq B \in \mathcal{O}'$ *for every conjunct* B *in* N.

Proof (sketch). It is easy to show that every axiom in $\mathcal{O}'$ is entailed by $\mathcal{O}$ since the inference rules in Table 3 derive only logical consequences of the axioms in their premises. In other words, the system of rules is sound. Therefore the "if" direction of points (i) and (ii) are trivial.

In order to prove the "only if" direction of points (i) and (ii), we construct a *canonical model* of $\mathcal{O}'$. Let Σ be the set of all conjunctions M such that $M \sqsubseteq \bot \notin \mathcal{O}'$. If Σ is empty, then $M \sqsubseteq \bot \in \mathcal{O}'$ for every M, and so, (i) and (ii) hold. In the remainder of the proof, we assume that Σ is not empty.

Let $\mathcal{I} = (\Delta^{\mathcal{I}}, \cdot^{\mathcal{I}})$ be such that $\Delta^{\mathcal{I}} = \Sigma^+$ is the set of all finite non-empty words over Σ, and $\cdot^{\mathcal{I}}$ defined as follows:

- $A^{\mathcal{I}} = \{wM \mid M \sqsubseteq A \in \mathcal{O}',\, w \in \Sigma^*\}$
- The roles are interpreted with smallest relations satisfying all role inclusions such that if $M \sqsubseteq \exists R.N \in \mathcal{O}'$ and $M \sqsubseteq \exists R.N' \notin \mathcal{O}'$ for every super-conjunct N' of N, then for every $w \in \Sigma^*$, either $\langle wM, w\rangle \in R^{\mathcal{I}}$ and $w \in A^{\mathcal{I}}$ for every $A \in N$, or otherwise $\langle wM, wMN\rangle \in R^{\mathcal{I}}$.

Intuitively, the interpretation $\mathcal{I}$ is a forest where nodes are labeled with non-contradictory conjunctions $M \in \Sigma$ and every node has a successor node for every non-contradictory conjunction $N \in \Sigma$. Roles can connect only successive nodes in such a way that all axioms $M \sqsubseteq \exists R.N \in \mathcal{O}'$ with maximal N are satisfied: if for a node marked with M the connection to its predecessor does not satisfy this axiom, it is connected to its successor marked with N. Rule **R3** ensures that N is not contradictory if M is not. Note that $\langle wM, wMN\rangle \in R^{\mathcal{I}}$ implies $M \sqsubseteq \exists R_1.N \in \mathcal{O}'$ for some $R_1 \sqsubseteq_{\mathcal{O}} R$. Below we demonstrate that $\mathcal{I}$ is a model of $\mathcal{O}$ (and consequently of $\mathcal{O}'$).

Claim 1 $wM \in \Sigma^+$ and $M \sqsubseteq C \in \mathcal{O}'$ imply $wM \in C^{\mathcal{I}}$.

- For $C = \bot$, if $M \sqsubseteq \bot \in \mathcal{O}'$ then $wM \notin \Sigma^+$.
- For $C = A$ the claim follows from the definition of $A^{\mathcal{I}}$.
- For $C = \exists R.B$, take $M \sqsubseteq \exists R.N \in \mathcal{O}'$ with the largest N containing B (it exists since $M \sqsubseteq \exists R.B \in \mathcal{O}'$). By definition of $R^{\mathcal{I}}$, we have $wM \in (\exists R.N)^{\mathcal{I}} \subseteq C^{\mathcal{I}}$.
- For $C = \forall R.B$, we show that: (i) $\langle wM, wMN\rangle \in R^{\mathcal{I}}$ implies $wMN \in B^{\mathcal{I}}$, and (ii) $\langle wNM, wN\rangle \in R^{\mathcal{I}}$ implies $wN \in B^{\mathcal{I}}$.

  In case (i) there is $M \sqsubseteq \exists R_1.N \in \mathcal{O}'$ with $R_1 \sqsubseteq_{\mathcal{O}} R$. Since $M \sqsubseteq C \in \mathcal{O}'$ and $\mathcal{O}'$ is closed under **R3**, we have $N = N \sqcap B$ (since N is a maximal conjunction), and so, $wMN \in B^{\mathcal{I}}$. In case (ii), there is $N \sqsubseteq \exists R_1.M \in \mathcal{O}'$ with $R_1 \sqsubseteq_{\mathcal{O}} R^-$. Since $M \sqsubseteq C \in \mathcal{O}'$ and $\mathcal{O}'$ is closed under **R4**, we have $N \sqsubseteq B \in \mathcal{O}'$, and so, $wN \in B^{\mathcal{I}}$.
- For $C = \leqslant 1 S.B$, we show that: (i) $\langle wM, wMN_i\rangle \in S^{\mathcal{I}}$ and $wMN_i \in B^{\mathcal{I}}$ for $i = 1, 2$ implies $N_1 = N_2$, and (ii) $\langle wNM, wN\rangle \in S^{\mathcal{I}}$, and $wN \in B^{\mathcal{I}}$ implies $\langle wNM, wNMN_1\rangle \notin S^{\mathcal{I}}$ whenever $wNMN_1 \in B^{\mathcal{I}}$.

  In case (i) we have $M \sqsubseteq \exists R_i.N_i \in \mathcal{O}'$ where $R_i \sqsubseteq_{\mathcal{O}} S$ and $N_i \sqsubseteq B \in \mathcal{O}'$, $i = 1, 2$. Since $\mathcal{O}'$ is closed under **R5**, we have $M \sqsubseteq \exists R_i.(N_1 \sqcap N_2) \in \mathcal{O}'$, $i = 1, 2$. Since each N_i is maximal for M and R_i, $i = 1, 2$, we have $N_1 = N_1 \sqcap N_2 = N_2$. In case (ii), we have $N \sqsubseteq \exists R.M \in \mathcal{O}'$, $R \sqsubseteq_{\mathcal{O}} S^-$, and $N \sqsubseteq B \in \mathcal{O}'$. Assume to the contrary that $\langle wNM, wNMN_1\rangle \in S^{\mathcal{I}}$ and $wNMN_1 \in B^{\mathcal{I}}$. Then $\langle wNM, wNMN_1\rangle \in R_1^{\mathcal{I}}$ for some $R_1 \sqsubseteq_{\mathcal{O}} S$ such that $M \sqsubseteq \exists R_1.N_1 \in \mathcal{O}'$, and $wNMN_1 \sqsubseteq B \in \mathcal{O}'$. Since $\mathcal{O}'$ is closed under **R6**, we have $N \sqsubseteq \exists R_1^-.M \in \mathcal{O}'$ and $N \sqsubseteq A \in \mathcal{O}$ for every conjunct A in N_1. Hence $M \sqsubseteq \exists R_1.N_1$ is already satisfied in wNM by its predecessor wN, and so the relation $\langle wNM, wNMN_1\rangle \in R_1^{\mathcal{I}}$ should not have been created.

Now for every axiom $\bigsqcap A_i \sqsubseteq C$ of form (n1) in $\mathcal{O}$, if $wM \in A_i^{\mathcal{I}}$ then $M \sqsubseteq A_i \in \mathcal{O}'$, and so, $M \sqsubseteq C \in \mathcal{O}'$ by **R1**. By Claim 1 we then have $wM \in C^{\mathcal{I}}$. Thus, $\mathcal{I}$ satisfies every axiom $\bigsqcap A_i \sqsubseteq C$ in $\mathcal{O}$ of form (n1). The definition of the interpretation of roles in $\mathcal{I}$ ensures that every role inclusion of form (n2) is also satisfied in $\mathcal{I}$. Hence, $\mathcal{I}$ is a model of $\mathcal{O}$.

Now we can finish the proof for the "only if" directions of points (i) and (ii). For proving (i), if $\mathcal{O} \models M \sqsubseteq B$ and $M \sqsubseteq \bot \notin \mathcal{O}'$ then for every $wM \in \Sigma^+$, we have $wM \in B^{\mathcal{I}}$ since $\mathcal{I}$ is a model of $\mathcal{O}$. Hence $M \sqsubseteq B \in \mathcal{O}'$ by definition of $\mathcal{I}$. For proving (ii), if $\mathcal{O} \models M \sqsubseteq \exists R.N$ and $M \sqsubseteq \bot \notin \mathcal{O}'$, then for $M \in \Sigma^+$, we have $M \in (\exists R.N)^{\mathcal{I}}$. Since $M \in \Sigma^+$ does not have a predecessor in Σ^+, there exists $M \sqsubseteq \exists R_1.N_1 \in \mathcal{O}'$ such that $R_1 \sqsubseteq_{\mathcal{O}} R$ and $MN_1 \in B^{\mathcal{I}}$ for every conjunct B in N. By definition of $\mathcal{I}$, this implies that $N_1 \sqsubseteq B \in \mathcal{O}'$ for every conjunct B in N. □

Theorem 4, in conjunction with Lemmas 2 and 3, implies that our procedure based on the rules in Table 3 can be used, in particular, for computing all subsumptions $A \sqsubseteq B$ between atomic concepts implied by the input ontology. In other words, the procedure is complete for classification of Horn $\mathcal{SHIQ}$ ontologies. Moreover, since the number of axioms of the form $M \sqsubseteq C$ and $M \sqsubseteq \exists R.N$ is at most exponential in the number of atomic concepts, the procedure is guaranteed to terminate in exponential time. Since deciding concept subsumptions in Horn $\mathcal{SHIQ}$ ontologies is ExpTime-complete (in ExpTime since Horn $\mathcal{SHIQ}$ is a fragment of $\mathcal{SHIQ}$ and ExpTime-hard since, e.g., Horn $\mathcal{SHIQ}$ contains $\mathcal{EL}$ with functionality), this implies that our procedure is computationally optimal.

4.5 Practical Considerations

Theorem 4 actually implies a stronger result than just completeness of the calculus for classification. The rules in Table 3 can, in fact, be used to derive all subsumptions between conjunctions of atomic concepts and (existentially restricted conjunctions of) atomic concepts. For computing just a subset of these relations, e.g., for classification, our procedure can be significantly optimized by applying rules **I1** and **I2** selectively depending on the goal subsumptions. Specifically, **I1** and **I2** can be restricted to produce conjunctions N only when either (i) N is the left hand side of a goal subsumption (e.g., for classification, N is an atomic concept from the input ontology), or (ii) an axiom of the form $M \sqsubseteq \exists R.N$ has been derived.

The above optimization not only reduces the number of inferences, but also yields a polynomial time classification procedure for $\mathcal{ELH}$ ontologies. Indeed, it is easy to see that for $\mathcal{ELH}$ ontologies the rules **R3**, **R5**, and **R6** never apply. The remaining rules produce only polynomially many axioms of the form $A \sqsubseteq C$ and $A \sqsubseteq \exists R.B$ since those rules (including **I1** and **I2**) never form conjunctions of several concepts.

5 Experimental Evaluation

The main goal for our consequence-based procedure for Horn $\mathcal{SHIQ}$ ontologies, was to reason efficiently with medium-sized ontologies such as Galen.[3] Galen turned out to be very difficult for model-building reasoners since it contains a large number of existential dependencies between classes of the form $A \sqsubseteq \exists R.B$. These dependencies are used, e.g., for expressing partonomy relations between anatomical units, for example: $\mathsf{BasilarArtery} \sqsubseteq \exists \mathsf{isBranchOf}.\mathsf{VertebralArtery}$. The dependency relation between classes induced by such axioms is very large and highly cyclic. Because of the numerous cycles, model building reasoners fail to produce (a finite representation of) a model since cycle detection mechanisms (blocking) do not appear to be effective in these cases.

The reasoner CEL for $\mathcal{EL}^+$ does not exhibit this problem since it does not build models but performs inferences according to Table 2. Axioms of the form $A \sqsubseteq \exists R.B$ are relatively harmless for CEL since these axioms alone do not result in any inference. Unfortunately, CEL cannot handle the full version of Galen since it does not support functionality and inverse roles, which Galen extensively uses. Thus the main question of our evaluation was whether the reasoner implemented according to the rules in Table 3 can scale well for ontologies outside the polynomial DL $\mathcal{EL}^+$.

To evaluate the performance of our procedure, we implemented a prototype reasoner CB[4] using a simplified version of the rules in Table 3 for Horn $\mathcal{SHIF}$ ontologies, which are sufficient for Galen. We compared the results with the model-building reasoners FaCT++ v.1.2.1,[5] Pellet v.1.5,[6] and HermiT v.0.9.3,[7] and the completion-based reasoner CEL v.1.0b.[8] We ran the experiments on a PC with a 2GHz Intel® Core™ Duo processor and 1.5GB RAM operated by Linux v.2.6.27 with Java VM v.1.6.0. We set time out of 3600 seconds and Java heap space of 1GB for Java-based reasoners.

We tested the classification of seven medical ontologies of various sizes and complexities. The Gene Ontology (GO)[9] and National Cancer Institute thesaurus (NCI)[10] are fairly big ontologies describing respectively 20465 and 27652 classes, but with a rather shallow structure inducing not many dependencies. We have considered four versions of Galen. GalenA with 2748 classes is based on an early version of Galen. GalenB with 23136 classes is based on a more recent version of Galen.[11] GalenA$^-$ and GalenB$^-$ are obtained from GalenA and GalenB by removing functionality and inverses. We have also included the results for a very large but simple ontology Snomed, which contains 389472 classes.

[3] http://www.opengalen.org/

[4] http://code.google.com/p/cb-reasoner/

[5] http://owl.man.ac.uk/factplusplus/

[6] http://clarkparsia.com/pellet/

[7] http://www.hermit-reasoner.com/

[8] http://lat.inf.tu-dresden.de/systems/cel/

[9] http://www.geneontology.org/

[10] http://www.cancer.gov/

[11] http://www.co-ode.org/galen/

	FaCT++	Pellet	HermiT	CEL	CB
GO	15.24	72.02	199.52	1.84	1.17
NCI	6.05	26.47	169.47	5.76	3.57
GalenA$^-$	3166.74	133.25	91.98	3.27	0.26
GalenA	465.35	—	45.72	*n/a*	0.32
GalenB$^-$	—	—	—	189.12	4.07
GalenB	—	—	—	*n/a*	9.58
Snomed	650.37	—	—	1185.70	49.44

Table 4: A comparison of classification times (in seconds): "—" means that the reasoner failed to return the result; "*n/a*" means that the test could not be performed.

The results of the experiments are summarized in Table 4. The time measured for CB includes loading, preprocessing, classification of the ontology and computing the transitively reduced and alphabetically sorted concept hierarchy. CB spends most of the time on loading for GO and NCI and on classification for the remaining ontologies, and considerably outperforms the other tested reasoners. In particular, CB is able to classify in just under 10 seconds the largest version of Galen, which could not be classified by the other reasoners.

It is worth commenting on the difference in the performance between CEL and CB. Although the rules in Table 3, when restricted to $\mathcal{EL}^+$ ontologies, are very similar to those in Table 2, there is a small but important difference. Namely, our procedure has no analogue of rule **CR4** in Table 2, which unfolds role inclusions into existential restrictions. Instead, the closure of role inclusions is computed separately and used in the premises of rules **R3**-**R6**. This strategy appears to be more efficient in situations when the number of role inclusions is small in comparison to the number of existential restrictions (which is mostly the case), and could explain the test results.

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