PRACTICAL USES OF EXISTENTIAL RULES IN KNOWLEDGE REPRESENTATION

Part 2: Existential Rules in Knowledge Representation

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Motivation

“Rules” are the epitome of symbolic reasoning:

- Many logical theories can be represented as rules
- Rules of inference are used to define deduction procedures

⇒ knowledge representation & reasoning as natural application area for existential rules

Goals for this part:

- Explain how to use rules to solve (quite unrelated) KRR problems
- Illustrate some useful modelling techniques
- Discuss aspects of reasoning performance
Description Logics

Description logics (DLs) are influential and widely used ontology languages

- basis of the W3C Web Ontology Language standard OWL
- specific DLs achieve good trade-offs between expressivity and complexity

**Schema modelling in DLs:** DLs talk about relational models that use only

- **classes** (unary predicates), e.g., “drink”
- **properties** (binary predicates), e.g., “madeWith”

DL ontologies describe relationships between these entities, such as

- **subclass relations**, e.g.,
  limeSyrup ⊑ fruitSyrup states that “every lime syrup is also a fruit syrup”
- **subproperty relations**, e.g.,
  madeWith ⊑ contains states that “if x is made with y, then x contains y”

→ DLs can model general terminological knowledge independent of specific facts
The DL $\mathcal{EL}^+\perp$ in a nutshell

The $\mathcal{EL}$ family of DLs is simple and supports polynomial time standard reasoning.

The DL $\mathcal{EL}^+\perp$ supports the following class expressions to describe derived classes:

- $\bot$ empty class (bottom) “the empty set”
- $\top$ universal class (top) “set of all elements”
- $\exists R.C$ existential restriction “set of all elements that have an $R$-relation to some element in class $C$”
- $C \cap D$ intersection “set of all elements that are in class $C$ and in class $D$”
The DL \( \mathcal{EL}^+ \) in a nutshell

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- \( C \cap D \) intersection “set of all elements that are in class \( C \) and in class \( D \)”

Class expressions and properties can be used in axioms:

- \( C \sqsubseteq D \) class subsumption “Every \( C \) is also a \( D \)”
- \( R \sqsubseteq S \) property subsumption “Every relation of type \( R \) is also one of type \( S \)”
- \( R \circ S \sqsubseteq T \) property chain “Elements connected by a chain of relations \( R \) followed by \( S \) are also directly connected by \( T \)”
All axioms of $\mathcal{EL}_+^\perp$ can be rewritten as existential rules

**Example:** The axiom

$$\text{alcoholicBeverage} \sqsubseteq \text{Drink} \sqcap \exists \text{contains. Alcohol}$$

can be written as a rule

$$\text{alcoholicBeverage}(x) \rightarrow \exists y. \text{Drink}(x) \wedge \text{contains}(x, y) \wedge \text{Alcohol}(y)$$
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can be written as a rule

$$\text{alcoholicBeverage}(x) \rightarrow \exists y. \text{Drink}(x) \land \text{contains}(x, y) \land \text{Alcohol}(y)$$

In general: this works for all Horn Description Logics

**Problem:** DLs are based on different reasoning methods. The rules they yield do often not lead to a terminating chase.
Example: A small $\mathcal{EL}^+_\bot$ ontology about drinks:

\[
\begin{align*}
\text{Highball} & \sqsubseteq \text{Drink} \sqcap \exists \text{madeWith}.\text{Spirit} \\
\text{Spirit} & \sqsubseteq \exists \text{contains}.\text{Alcohol} \\
\text{Drink} & \sqcap \exists \text{contains}.\text{Alcohol} \sqsubseteq \text{alcoholicBeverage} \\
\text{madeWith} \circ \text{contains} & \sqsubseteq \text{contains}
\end{align*}
\]

From this example, we should be able to conclude Highball $\sqsubseteq$ alcoholicBeverage.

Definition: The task of computing all logically entailed subsumptions $A \sqsubseteq B$ between atomic classes $A$ and $B$ is called classification.

Classification for $\mathcal{EL}^+_\bot$ is polynomial, but how exactly should we compute it in rules?
Published: 17 November 2013

The Incredible ELK

From Polynomial Procedures to Efficient Reasoning with $\mathcal{EL}$ Ontologies

Yevgeny Kazakov, Markus Krötzsch & František Simančík

*Journal of Automated Reasoning* 53, 1–61 (2014) | Cite this article

518 accesses | 93 citations | Metrics
Prior research . . .

Fig. 3 Optimized inference rules for classification of $\mathcal{EL}^+_{\Perp}$ ontologies
How to read such rules

General form of the rules:

\[
\text{rule name } \frac{\text{pre-condition}}{\text{conclusion}} : \text{ side condition}
\]

For example:

\[
R^+_{\sqcap} \frac{C \sqsubseteq D_1 \quad C \sqsubseteq D_2}{C \sqsubseteq D_1 \sqcap D_2} : D_1 \sqcap D_2 \text{ occur negatively in } \mathcal{O}
\]

where the parts have the following meaning:

- \( O \): the given \( \mathcal{EL}^+_{\sqcap} \) ontology
- \( C, D_1, D_2 \): arbitrary (possibly nested) \( \mathcal{EL}^+_{\sqcap} \) class expressions
- “to occur negatively”: to appear in a subclass position
Encoding a calculus in rules

\[
\begin{align*}
R_0 & \quad \frac{\text{init}(C)}{C \sqsubseteq C} \\
R_T & \quad \frac{\text{init}(C)}{C \sqsubseteq \top} : \top \text{ occurs negatively in } \mathcal{O} \\
R_\sqcap & \quad \frac{C \sqsubseteq D_1 \sqcap D_2}{C \sqsubseteq D_1 \quad C \sqsubseteq D_2} : D_1 \sqcap D_2 \text{ occur negatively in } \mathcal{O} \\
R_\exists & \quad \frac{E \sqsubseteq \exists R.C}{E \xrightarrow{R} C} \\
R_\exists^+ & \quad \frac{E \xrightarrow{R} C \quad C \sqsubseteq D}{E \sqsubseteq \exists S.D} : \exists S.D \text{ occurs negatively in } \mathcal{O} \\
R_\sqsubseteq & \quad \frac{C \sqsubseteq D}{D \sqsubseteq E \in \mathcal{O}} \\
R_\sqsupset & \quad \frac{E \xrightarrow{R_1} C \quad C \xrightarrow{R_2} D}{E \xrightarrow{S} D} : \begin{array}{c}
R_1 \sqsubseteq^* S_1 \\
R_2 \sqsubseteq^* S_2 \\
S_1 \cup S_2 \sqsubseteq S \in \mathcal{O}
\end{array} \\
R_{\text{init}} & \quad \frac{}{\text{init}(C)}
\end{align*}
\]

**Fig. 3** Optimized inference rules for classification of $\mathcal{EL}^+_\bot$ ontologies
Encoding a calculus in rules

Three different types of inferences

Fig. 3 Optimized inference rules for classification of $\mathcal{EL}^+_{\bot}$ ontologies
Encoding a calculus in rules

Three different types of inferences

$R_0 \frac{\text{init}(C)}{C \sqsubseteq C}$

$R_\top \frac{\text{init}(C)}{C \sqsubseteq \top}$

$\frac{C \sqsubseteq D_1 \sqcap D_2}{C \sqsubseteq D_1} \quad \frac{C \sqsubseteq D_2}{C \sqsubseteq D_2}$

$R^- \frac{C \sqsubseteq D_1 \sqcap D_2}{C \sqsubseteq D_1 \sqcap D_2}$

$R_\cap \frac{E \sqsubseteq \exists R.C}{E \sqsubseteq R.C}$

$R_\cap \frac{E \sqsubseteq \exists S.D}{E \sqsubseteq \exists S.D}$

$R_\cap \frac{E \sqsubseteq C \quad C \sqsubseteq D}{E \sqsubseteq C \sqcap D}$

Four kinds of side conditions

$R_\cap \frac{E \sqsubseteq \exists S.D}{\exists S.D \text{ occurs negatively in } O}$

$R_\cap \frac{E \sqsubseteq C \quad C \sqsubseteq D}{E \sqsubseteq C \sqcap D}$

$R_\cap \frac{E \sqsubseteq C \quad C \sqsubseteq D}{E \sqsubseteq C \sqcap D}$

$R_\cap \frac{E \sqsubseteq C \quad C \sqsubseteq D}{E \sqsubseteq C \sqcap D}$

$R_\cap \frac{E \sqsubseteq C \quad C \sqsubseteq D}{E \sqsubseteq C \sqcap D}$

Fig. 3 Optimized inference rules for classification of $\mathcal{EL}^+_{\bot}$ ontologies
We simply turn every expression in the calculus into a fact:

<table>
<thead>
<tr>
<th>Expression in calculus</th>
<th>Encoding in Datalog facts</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C$ occurs negatively in $O$</td>
<td>nf:isSubClass($C$)</td>
</tr>
<tr>
<td>$C \sqsubseteq D \in O$</td>
<td>nf:subClassOf($C$, $D$)</td>
</tr>
<tr>
<td>$R \sqsubseteq^* S$</td>
<td>nf:subPro0f($R$, $S$)</td>
</tr>
<tr>
<td>$S_1 \circ S_2 \sqsubseteq S$</td>
<td>nf:subPropChain($S_1$, $S_2$, $S$)</td>
</tr>
<tr>
<td>$C \sqsubseteq D$</td>
<td>inf:subClass0f($C$, $D$)</td>
</tr>
<tr>
<td>$E \xrightarrow{R} C$</td>
<td>inf:ex($E$, $R$, $C$)</td>
</tr>
<tr>
<td>init($C$)</td>
<td>inf:init($C$)</td>
</tr>
</tbody>
</table>
We also need to encode the structure of class expressions.
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We use an obvious encoding where every sub-expression becomes a fact.

**Example:** The class $A \sqinter \exists R. (B \sqinter C)$ is encoded by facts

```plaintext
nf:conj("A \sqinter \exists R. (B \sqinter C)", A, "\exists R. (B \sqinter C)"

nf:exists("\exists R. (B \sqinter C)", R, "B \sqinter C"

nf:conj("B \sqinter C", B, C)
```

where every sub-expression is represented by a constant.

Expressions $\top$ and $\bot$ are encoded by their special OWL names `owl:Thing` and `owl:Nothing`. 
### Encoding expressions in predicates

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<tr>
<td>( \top )</td>
<td>owl:Thing</td>
</tr>
<tr>
<td>( \bot )</td>
<td>owl:Nothing</td>
</tr>
<tr>
<td>( X = \exists R.C )</td>
<td>nf:exists((X,R,C))</td>
</tr>
<tr>
<td>( X = C \cap D )</td>
<td>nf:conj((X,C,D))</td>
</tr>
<tr>
<td>( C ) occurs negatively in ( O )</td>
<td>nf:isSubClass((C))</td>
</tr>
<tr>
<td>( C \sqsubseteq D \in O )</td>
<td>nf:subClassOf((C,D))</td>
</tr>
<tr>
<td>( R \sqsubseteq^* S )</td>
<td>nf:subProp0f((R,S))</td>
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<tr>
<td>( S_1 \circ S_2 \sqsubseteq S )</td>
<td>nf:subPropChain((S_1,S_2,S))</td>
</tr>
<tr>
<td>( C \sqsubseteq D )</td>
<td>inf:subClassOf((C,D))</td>
</tr>
<tr>
<td>( E \stackrel{R}{\rightarrow} C )</td>
<td>inf:ex((E,R,C))</td>
</tr>
<tr>
<td>init((C))</td>
<td>inf:init((C))</td>
</tr>
</tbody>
</table>
Encoding calculus rules in Datalog

Now all rules from the paper can simply be transcoded

Example:

\[
\begin{align*}
\mathcal{R}_\Pi^+ & \quad \frac{C \sqsubseteq D_1 \quad C \sqsubseteq D_2}{C \sqsubseteq D_1 \cap D_2} : D_1 \cap D_2 \text{ occur negatively in } \mathcal{O}
\end{align*}
\]

becomes

\[
\begin{align*}
\inf:\text{subClassOf}(\text{?C}, \text{?D1andD2}) & : - \\
\inf:\text{subClassOf}(\text{?C}, \text{?D1}), \inf:\text{subClassOf}(\text{?C}, \text{?D2}), \\
\text{nf:conj}(\text{?D1andD2}, \text{?D1}, \text{?D2}), \text{nf:isSubClass}(\text{?D1andD2})
\end{align*}
\]
Steps to produce the Datalog rules:

1. Read the paper carefully and understand the rule structure
2. Define predicates to encode the relevant expressions
3. Rewrite the rules in the new language

Steps to classify an ontology:

1. Encode the ontology using facts for the nf: predicates
2. Store the facts in an rls file, or in csv files
3. Evaluate this data with the calculus rules
4. Computed subclass relations are in predicate inf:subClassOf
Let’s classify the Galen ontology (EL version)

(1) @clear ALL . (if still running)

(2) Register normalised Galen sources and load calculus:
   @load "el/galen-sources.rls" .
   @load "el/elk-calculus.rls" .

(3) @reason .

(4) Try some queries:
   @query COUNT mainSubClassOf(?A,?B) .
   @query mainSubClassOf(?A,galen:Virus) .

(5) Export classification to file:
   @query mainSubClassOf(?A,?B) EXPORTCSV "galen-inf-subclass.csv" .
Performance tuning

Performance is ok for a first translation, but could be improved . . .

. . . but effective tuning requires knowledge of the reasoner!
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. . . but effective tuning requires knowledge of the reasoner!

Special aspects of VLog:

• Predicate tuples are indexed in their given order
  
  

• Body conjunctions are evaluated using binary joins

• Join order is determined by heuristics (esp. predicate size)
  
  Fast: short bodies; selective binary joins
  
  Slow: long bodies; possibly very un-selective joins

Running in VLog in debug-mode can yield insights on slow rule executions.
Some rules are hard to process:

\[
\]
Performance tuning 1: Decompose rules

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\[
\]

Likely bad join order (starting from small predicates):

\[
\]

But most ontologies have very few properties (?R, ?S), each used in a large part of the existential restrictions \( \sim \) essentially a product \( \text{nf:exists}(?Y, ?S, ?D) \times \text{inf:ex}(?E, ?R, ?C) \)
Performance tuning 1: Decompose rules

Some rules are hard to process:

\[
\text{inf:subClassOf}(\text{?E}, \text{?Y}) :- \text{inf:ex}(\text{?E}, \text{?R}, \text{?C}), \text{inf:subClassOf}(\text{?C}, \text{?D}), \\
\text{nf:subProp}(\text{?R}, \text{?S}), \text{nf:exists}(\text{?Y}, \text{?S}, \text{?D}), \text{nf:isSubClass}(\text{?Y}) .
\]

Likely bad join order (starting from small predicates):

\[
(\text{nf:exists}(\text{?Y}, \text{?S}, \text{?D}) \bowtie \text{nf:subProp}(\text{?R}, \text{?S})) \bowtie \text{inf:ex}(\text{?E}, \text{?R}, \text{?C})
\]

But most ontologies have very few properties (\text{?R}, \text{?S}), each used in a large part of the existential restrictions \( \sim \) essentially a product \( \text{nf:exists}(\text{?Y}, \text{?S}, \text{?D}) \times \text{inf:ex}(\text{?E}, \text{?R}, \text{?C}) \)

Solution: Replace problematic rule by several rules:

\[
\text{subExt}(\text{?D}, \text{?R}, \text{?Y}) :- \text{nf:subProp}(\text{?R}, \text{?S}), \text{nf:exists}(\text{?Y}, \text{?S}, \text{?D}), \\
\text{nf:isSubClass}(\text{?Y}) .
\]

\[
\text{aux}(\text{?C}, \text{?R}, \text{?Y}) :- \text{inf:subClassOf}(\text{?C}, \text{?D}), \text{subExt}(\text{?D}, \text{?R}, \text{?Y}) .
\]

\[
\text{inf:subClassOf}(\text{?E}, \text{?Y}) :- \text{inf:ex}(\text{?E}, \text{?R}, \text{?C}), \text{aux}(\text{?C}, \text{?R}, \text{?Y}) .
\]
Argument order in derived predicates can be changed:

\[
\]
Performance tuning 2: Argument order

Argument order in derived predicates can be changed:

```
inf:subClassOf(?E,?Y) :- inf:ex(?E,?R,?C), aux(?C,?R,?Y).
```

For this rule, it would work better if we flipped the order of `inf:ex`:

```
infsubClassOf(?E,?Y) :- inf:xe(?C,?R,?E), aux(?C,?R,?Y).
```

Of course, this must be done across all rules!
Performance tuning 2: Argument order

**Argument order in derived predicates can be changed:**

```
inf:subClassOf(?E,?Y) :- inf:ex(?E,?R,?C), aux(?C,?R,?Y) .
```

For this rule, it would work better if we flipped the order of `inf:ex`:

```
```

Of course, this must be done across all rules!

An optimised version of the calculus is in file `el/elk-caclulus-optimised.rls`. Try it with Galen.

**General guideline:** There is no simple rule for how to improve performance, since many optimisations interact. Try what works best.

(The fastest results come from making typos: be sure to check correctness, too!)
Normalisation

The calculus requires us to pre-compute facts for the ontology encoding

- Standard libraries like the OWL API for Java can help
- But it still requires another software tool
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Can’t we do this in rules, too?

Rationale:

- OWL (DL) ontologies are typically stored in an RDF encoding
- Rulewerk and VLog can read RDF data natively
- Rules can perform structural transformations
The RDF format describes labelled graphs, and DL axioms are encoded in graphs as well.

**The following graph encodes** $A \sqsubseteq \exists R. (B \sqcap C)$:
Observation: OWL/RDF contains enough auxiliary nodes to use to represent subexpressions!
Extracting $\mathcal{EL}$ from RDF

**Observation:** OWL/RDF contains enough auxiliary nodes to use to represent subexpressions!

Making suitable rules is not hard:

- **Extracting** $C \sqsubseteq D$:

  \[
  \text{nf:subClassOf}(\text{?C}, \text{?D}) :- \text{TRIPLE}(\text{?C}, \text{rdfs:subClassOf}, \text{?D}) .
  \]

- **Extracting** $\exists R.X$:

  \[
  \text{nf:exists}(\text{?X}, \text{?R}, \text{?C}) :- \text{TRIPLE}(\text{?X}, \text{owl:someValuesFrom}, \text{?C}), \\
  \text{TRIPLE}(\text{?X}, \text{owl:onProperty}, \text{?R}) .
  \]

- **Extracting** binary $B \sqcap C$:

  \[
  \text{ex:conj}(\text{?X}, \text{?B}, \text{?C}) :- \\
  \text{TRIPLE}(\text{?X}, \text{owl:intersectionOf}, \text{?L1}), \\
  \text{TRIPLE}(\text{?L1}, \text{rdf:next}, \text{?L2}), \text{TRIPLE}(\text{?L2}, \text{rdf:next}, \text{rdf:nil}), \\
  \text{TRIPLE}(\text{?L1}, \text{rdf:first}, \text{?B}), \text{TRIPLE}(\text{?L2}, \text{rdf:first}, \text{?C}) .
  \]

The general case requires some more rules, since OWL encodes n-ary conjunctions as linked lists.

Markus Krötzsch, 4 September 2020

Practical Uses of Existential Rules in Knowledge Representation
Reusing sub-expressions

**Problem:** The same class expression can occur thousands of times in one ontology
\[ \Rightarrow \] duplicated structures, which will all be inferred to be equivalent!
Reusing sub-expressions

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\[ \rightarrow \text{duplicated structures, which will all be inferred to be equivalent!} \]

**Solution:** Replace auxiliary nodes by new elements, unique for each expression
Reusing sub-expressions

Problem: The same class expression can occur thousands of times in one ontology $\leadsto$ duplicated structures, which will all be inferred to be equivalent!

Solution: Replace auxiliary nodes by new elements, unique for each expression

Approach:

- Mark the “main classes” that are not used in auxiliary positions (using negation)
- Use auxiliary predicates for syntactic extraction, e.g.:
  \[
  \text{synEx}(\text{?X}, \text{?R}, \text{?C}) : - \ \text{TRIPLE}(\text{?X}, \text{owl:someValuesFrom}, \text{?C}), \\
  \text{TRIPLE}(\text{?X}, \text{owl:onProperty}, \text{?R}) .
  \]
- Create and define representatives for every expression, recursively:
  \[
  \text{repOf}(\text{?X}, \text{?X}) : - \ \text{nf:isMainClass}(\text{?X}) .
  \]
  \[
  \text{synExRep}(\text{?X}, \text{?R}, \text{?Rep}) : - \ \text{synEx}(\text{?X}, \text{?R}, \text{?Y}), \ \text{repOf}(\text{?Y}, \text{?Rep}) .
  \]
  \[
  \text{nf:exists}(\text{?New}, \text{?R}, \text{?Rep}) : - \ \text{synExRep}(\text{?X}, \text{?R}, \text{?Rep}) .
  \]
  \[
  \text{repOf}(\text{?X}, \text{?N}) : - \ \text{synExRep}(\text{?X}, \text{?R}, \text{?Rep}), \ \text{nf:exists}(\text{?N}, \text{?R}, \text{?Rep}) .
  \]
Hands-On #5: Normalising Galen

Rules for OWL $\mathcal{EL}$ normalisation are given in el/elk-normalisation.rls

Steps to normalise Galen EL from OWL/RDF

1. \texttt{@clear ALL}  . (if still running)

2. Load Galen from RDF:
   \texttt{@load RDF "el/galen-el.rdf"}  .

3. Load the normalisation rules:
   \texttt{@load "el/elk-normalisation.rls"}  .

4. \texttt{@reason}  .

5. Check result, e.g.,
   \texttt{@query nf:exists(?X,?R,?C) LIMIT 10}  .

6. Export normalised facts to CSV, e.g.,
   \texttt{@query nf:subClassOf(?C,?D) EXPORTCSV "my-galen-subClassOf.csv"}  .
Putting it all together

We have just implemented a complete $\mathcal{EL}$ reasoner in 46 existential rules: just load `elk-normalisation.rls` and `elk-calculus-optimised.rls` together with the triples of a OWL/RDF file!

How about performance?

- Running normalisation and reasoning separately is faster than doing everything in one step (more rules – harder to optimise for VLog)
- Performance is below dedicated OWL EL reasoners, but practical:
  - [Laptop, Intel i7 2.70GHz, 4G Java heap]
  - Normalisation only: 2.5sec
  - Reasoning only: 25sec
  - All in one: 4min

But then again, this only took <50 lines of code!

Markus Krötzsch, 4 September 2020
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<tr>
<td>GALEN EL (250K triples)</td>
<td>2.5sec</td>
<td>25sec</td>
</tr>
<tr>
<td>SNOMED CT (2.9M triples)</td>
<td>30sec</td>
<td>2min</td>
</tr>
</tbody>
</table>

But then again, this only took <50 lines of code!
What we learned

- Many rules-based reasoning calculi can be implemented in rules
- This is a multi-step process:
  - Develop suitable encoding
  - Translate and debug rules
  - Optimise performance
- Rules also help with related tasks (normalisation, reduction, result comparison, …)
- Rulewerk/VLog can be used for rapid prototyping of reasoning calculi

Up next: how to handle reasoning tasks beyond P
References

Current main reference for Rulewerk (formerly: VLog4j)


