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

$\leadsto$ 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 $\sqsubseteq$ fruitSyrup states that “every lime syrup is also a fruit syrup”
- subproperty relations, e.g.,
  madeWith $\sqsubseteq$ contains states that “if x is made with y, then x contains y”

$\rightsquigarrow$ DLs can model general terminological knowledge independent of specific facts

The DL $\mathcal{EL}_\bot^+$ in a nutshell

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

The DL $\mathcal{EL}_\bot^+$ 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”
$C \sqcap D$	intersection	“set of all elements that are in class C and in class D”

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:

$\perp$	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"
$C \sqcap D$	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"

$\mathcal{EL}^{+}_{\perp}$ and existential rules

All axioms of $\mathcal{EL}^{+}_{\perp}$ can be rewritten as existential rules

Example: The axiom

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

can be written as a rule

$$\mathsf{alcoholicBeverage}(x) \to \exists y.\mathsf{Drink}(x) \wedge \mathsf{contains}(x, y) \wedge \mathsf{Alcohol}(y)$$

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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.

Reasoning for DLs

Example: A small $\mathcal{EL}_\bot^+$ ontology about drinks:

$$\begin{aligned}
\mathsf{Highball} &\sqsubseteq \mathsf{Drink} \sqcap \exists \mathsf{madeWith}.\mathsf{Spirit} \\
\mathsf{Spirit} &\sqsubseteq \exists \mathsf{contains}.\mathsf{Alcohol} \\
\mathsf{Drink} \sqcap \exists \mathsf{contains}.\mathsf{Alcohol} &\sqsubseteq \mathsf{alcoholicBeverage} \\
\mathsf{madeWith} \circ \mathsf{contains} &\sqsubseteq \mathsf{contains}
\end{aligned}$$

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

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?

Prior research . . .

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

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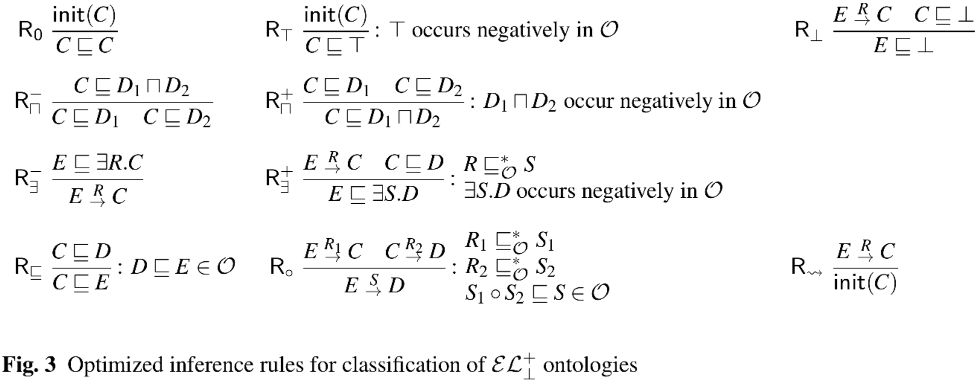


$$\mathsf{R}_0\ \frac{\mathsf{init}(C)}{C \sqsubseteq C} \qquad \mathsf{R}_\top\ \frac{\mathsf{init}(C)}{C \sqsubseteq \top} : \top \text{ occurs negatively in } \mathcal{O} \qquad \mathsf{R}_\bot\ \frac{E \xrightarrow{R} C \quad C \sqsubseteq \bot}{E \sqsubseteq \bot}$$

$$\mathsf{R}^-_\sqcap\ \frac{C \sqsubseteq D_1 \sqcap D_2}{C \sqsubseteq D_1 \quad C \sqsubseteq D_2} \qquad \mathsf{R}^+_\sqcap\ \frac{C \sqsubseteq D_1 \quad C \sqsubseteq D_2}{C \sqsubseteq D_1 \sqcap D_2} : D_1 \sqcap D_2 \text{ occur negatively in } \mathcal{O}$$

$$\mathsf{R}^-_\exists\ \frac{E \sqsubseteq \exists R.C}{E \xrightarrow{R} C} \qquad \mathsf{R}^+_\exists\ \frac{E \xrightarrow{R} C \quad C \sqsubseteq D}{E \sqsubseteq \exists S.D} : \begin{array}{l} R \sqsubseteq^*_\mathcal{O} S \\ \exists S.D \text{ occurs negatively in } \mathcal{O} \end{array}$$

$$\mathsf{R}_\sqsubseteq\ \frac{C \sqsubseteq D}{C \sqsubseteq E} : D \sqsubseteq E \in \mathcal{O} \qquad \mathsf{R}_\circ\ \frac{E \xrightarrow{R_1} C \quad C \xrightarrow{R_2} D}{E \xrightarrow{S} D} : \begin{array}{l} R_1 \sqsubseteq^*_\mathcal{O} S_1 \\ R_2 \sqsubseteq^*_\mathcal{O} S_2 \\ S_1 \circ S_2 \sqsubseteq S \in \mathcal{O} \end{array} \qquad \mathsf{R}_\leadsto\ \frac{E \xrightarrow{R} C}{\mathsf{init}(C)}$$

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

How to read such rules

General form of the rules:

$$\text{rule name} \quad \frac{\text{pre-condition}}{\text{conclusion}} : \text{side condition}$$

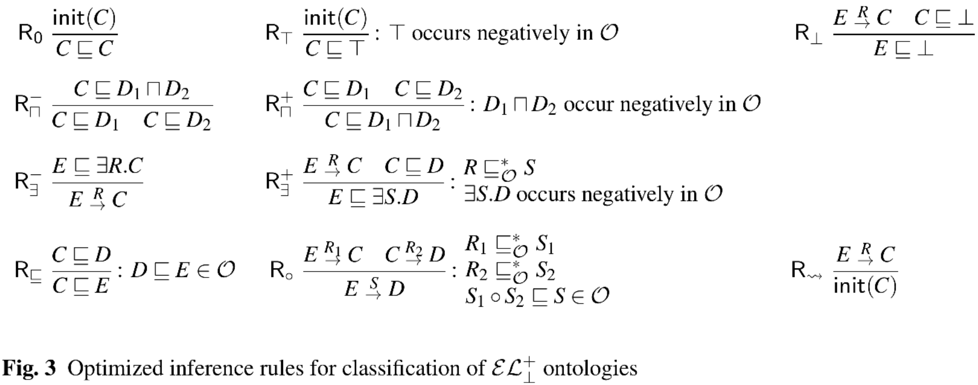
For example:

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

where the parts have the following meaning:

- $\mathcal{O}$: the given $\mathcal{EL}^{+}_{\bot}$ ontology
- C, D_1, D_2: arbitrary (possibly nested) $\mathcal{EL}^{+}_{\bot}$ class expressions
- "to occur negatively": to appear in a subclass position

Encoding a calculus in rules



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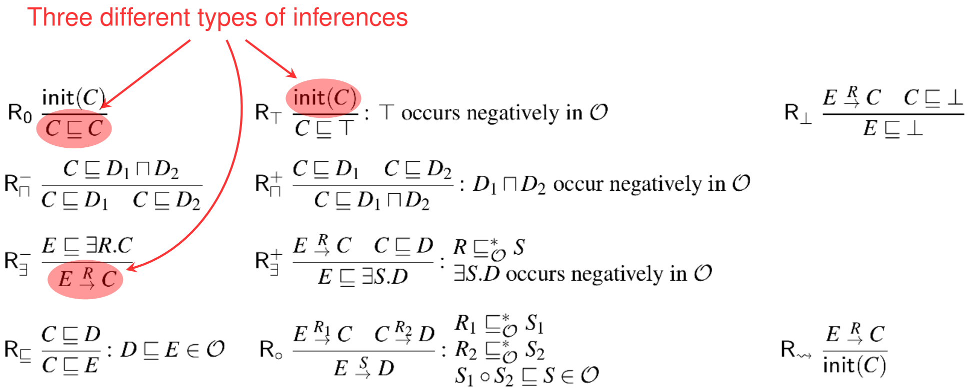

Three different types of inferences

$$\mathsf{R}_0\ \frac{\mathsf{init}(C)}{C \sqsubseteq C} \qquad \mathsf{R}_\top\ \frac{\mathsf{init}(C)}{C \sqsubseteq \top} : \top \text{ occurs negatively in } \mathcal{O} \qquad \mathsf{R}_\bot\ \frac{E \xrightarrow{R} C \quad C \sqsubseteq \bot}{E \sqsubseteq \bot}$$

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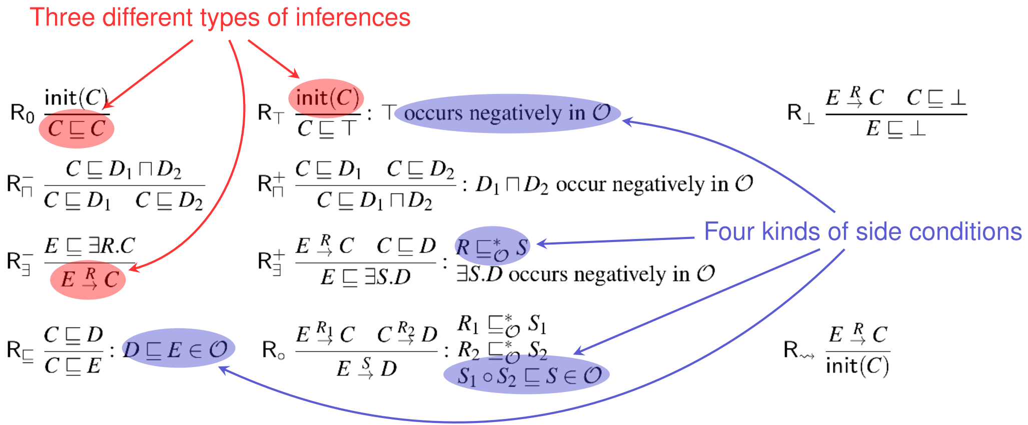

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Encoding expressions in predicates

We simply turn every expression in the calculus into a fact:

Expression in calculus	**Encoding in Datalog facts**
C occurs negatively in $\mathcal{O}$	`nf:isSubClass(`C`)`
$C \sqsubseteq D \in \mathcal{O}$	`nf:subClassOf(`C`,`D`)`
$R \sqsubseteq^*_{\mathcal{O}} S$	`nf:subProOf(`R`,`S`)`
$S_1 \circ S_2 \sqsubseteq S$	`nf:subPropChain(`S_1`,`S_2`,`S`)`
$C \sqsubseteq D$	`inf:subClassOf(`C`,`D`)`
$E \xrightarrow{R} C$	`inf:ex(`E`,`R`,`C`)`
init(C)	`inf:init(`C`)`

Encoding class expressions

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 $A \sqcap \exists R.(B \sqcap C)$ is encoded by facts

$$\texttt{nf:conj(}"A \sqcap \exists R.(B \sqcap C)"\texttt{,}A\texttt{,}"\exists R.(B \sqcap C)"\texttt{)}$$

$$\texttt{nf:exists(}"\exists R.(B \sqcap C)"\texttt{,}R\texttt{,}"B \sqcap C"\texttt{)}$$

$$\texttt{nf:conj(}"B \sqcap C"\texttt{,}B\texttt{,}C\texttt{)}$$

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

Expression in calculus	**Encoding in Datalog facts**
$\top$	`owl:Thing`
$\bot$	`owl:Nothing`
$X = \exists R.C$	`nf:exists(`X`,`R`,`C`)`
$X = C \sqcap D$	`nf:conj(`X`,`C`,`D`)`
C occurs negatively in $\mathcal{O}$	`nf:isSubClass(`C`)`
$C \sqsubseteq D \in \mathcal{O}$	`nf:subClassOf(`C`,`D`)`
$R \sqsubseteq^*_{\mathcal{O}} S$	`nf:subProOf(`R`,`S`)`
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$C \sqsubseteq D$	`inf:subClassOf(`C`,`D`)`
$E \xrightarrow{R} C$	`inf:ex(`E`,`R`,`C`)`
init(C)	`inf:init(`C`)`

Encoding calculus rules in Datalog

Now all rules from the paper can simply be transcoded

Example:

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

becomes

```
inf:subClassOf(?C,?D1andD2) :-
    inf:subClassOf(?C,?D1), inf:subClassOf(?C,?D2),
    nf:conj(?D1andD2,?D1,?D2), nf:isSubClass(?D1andD2) .
```

Bringing it all together

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`

Hands-On #4: Classifying Galen-EL

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
  Fast: `p(?X,?Y,?Z), q(?X,?Y,?V)`
  Slow: `p(?Z,?Y,?X), q(?V,?X,?Y)`
- 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.

Performance tuning 1: Decompose rules

Some rules are hard to process:

```
inf:subClassOf(?E,?Y) :- inf:ex(?E,?R,?C), inf:subClassOf(?C,?D),
      nf:subProp(?R,?S), nf:exists(?Y,?S,?D), nf:isSubClass(?Y) .
```

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```

Likely bad join order (starting from small predicates):

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

But most ontologies have very few properties (`?R`, `?S`), each used in a large part of the existential restrictions ⇝ essentially a product `nf:exists(?Y,?S,?D)` × `inf:ex(?E,?R,?C)`

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Solution: Replace problematic rule by several rules:

```
     subExt(?D,?R,?Y) :- nf:subProp(?R,?S), nf:exists(?Y,?S,?D),
                         nf:isSubClass(?Y) .
        aux(?C,?R,?Y) :- inf:subClassOf(?C,?D), subExt(?D,?R,?Y) .
inf:subClassOf(?E,?Y) :- inf:ex(?E,?R,?C), aux(?C,?R,?Y) .
```

Performance tuning 2: Argument order

Argument order in derived predicates can be changed:

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

```
inf:subClassOf(?E,?Y) :- inf:xe(?C,?R,?E), aux(?C,?R,?Y) .
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Of course, this must be done across all rules!

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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
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Can’t we do this in rules, too?

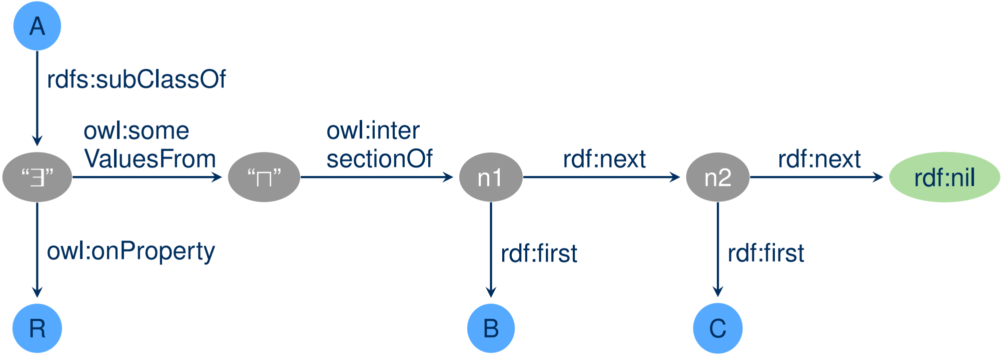
Rationale:

- OWL (DL) ontologies are typically stored in an RDF encoding
- Rulewerk and VLog can read RDF data natively
- Rules can perform structural transformations

$\mathcal{EL}$ in RDF

The RDF format describes labelled graphs, and DL axioms are encoded in graphs as well.

The following graph encodes $A \sqsubseteq \exists R.(B \sqcap C)$**:**



Extracting $\mathcal{EL}$ from RDF

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

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Making suitable rules is not hard:

- Extracting $C \sqsubseteq D$:

```
nf:subClassOf(?C,?D) :- TRIPLE(?C, rdfs:subClassOf, ?D) .
```

- Extracting $\exists R.X$:

```
nf:exists(?X,?R,?C) :- TRIPLE(?X, owl:someValuesFrom, ?C),
                       TRIPLE(?X, owl:onProperty, ?R) .
```

- Extracting binary $B \sqcap C$:

```
ex:conj(?X,?B,?C) :-
    TRIPLE(?X, owl:intersectionOf, ?L1),
    TRIPLE(?L1,rdf:next,?L2), TRIPLE(?L2,rdf:next,rdf:nil),
    TRIPLE(?L1,rdf:first,?B), TRIPLE(?L2,rdf:first,?C) .
```

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

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!

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Approach:

- Mark the “main classes” that are not used in auxiliary positions (using negation)
- Use auxiliary predicates for syntactic extraction, e.g.:

```
synEx(?X,?R,?C) :- TRIPLE(?X, owl:someValuesFrom, ?C),
                   TRIPLE(?X, owl:onProperty, ?R) .
```

- Create and define representatives for every expression, recursively:

```
          repOf(?X,?X) :- nf:isMainClass(?X) .
   synExRep(?X,?R,?Rep) :- synEx(?X,?R,?Y), repOf(?Y,?Rep) .
nf:exists(!New,?R,?Rep) :- synExRep(?X,?R,?Rep) .
          repOf(?X,?N) :- synExRep(?X,?R,?Rep), nf:exists(?N,?R,?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. `@clear ALL .` (if still running)
2. Load Galen from RDF:
   ```
   @load RDF "el/galen-el.rdf" .
   ```
3. Load the normalisation rules:
   ```
   @load "el/elk-normalisation.rls" .
   ```
4. `@reason .`
5. Check result, e.g.,
   ```
   @query nf:exists(?X,?R,?C) LIMIT 10 .
   ```
6. Export normalised facts to CSV, e.g.,
   ```
   @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!

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	Reasoning only	All in one
GALEN EL (250K triples)	2.5sec	25sec	4min
SNOMED CT (2.9M triples)	30sec	2min	9min

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

Summary

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

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[2] David Carral, Irina Dragoste, Markus Krötzsch: **Reasoner = Logical Calculus + Rule Engine.** KI - Künstliche Intelligenz, 2020. Further discussion of this use case (rules for reasoning)

[3] Yevgeny Kazakov, Markus Krötzsch, Frantisek Simancik: **The Incredible ELK – From Polynomial Procedures to Efficient Reasoning with $\mathcal{EL}$ Ontologies.** J. Autom. Reason. 53(1): 1-61 (2014) Source of the DL reasoning calculus used herein

[4] Markus Krötzsch: **Efficient Rule-Based Inferencing for OWL EL.** IJCAI 2011: 2668-2673 An earlier, less efficient Datalog calculus for $\mathcal{EL}$

[5] Jacopo Urbani, Ceriel J. H. Jacobs, Markus Krötzsch: **Column-Oriented Datalog Materialization for Large Knowledge Graphs.** AAAI 2016: 258-264 Original publication about VLog's design; explains the indexing method relevant for our optimisation here