Dresden University of Technology
Faculty of Computer Science

TECHNISCHE UNIVERSITÄT DRESDEN

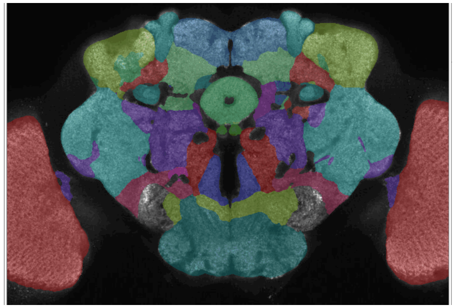
Existential Rules in Ontological Modelling

Markus Krötzsch
Dresden University of Technology

November 20, 2013

Rules and Ontologies

- Ontologies
  - Structural models
  - Static
  - Output known at design time



- Rules
  - Computational models
  - Dynamic
  - Problem solving at runtime

Rules in Computation

- Logic programming
  - PROLOG, Answer Set Programming
- Data access and query languages
  - Datalog
- Information integration and data exchange
  - Database Dependencies and Constraints
- Derivation
  - Deduction Rules, Production Rules

Two Unknowns

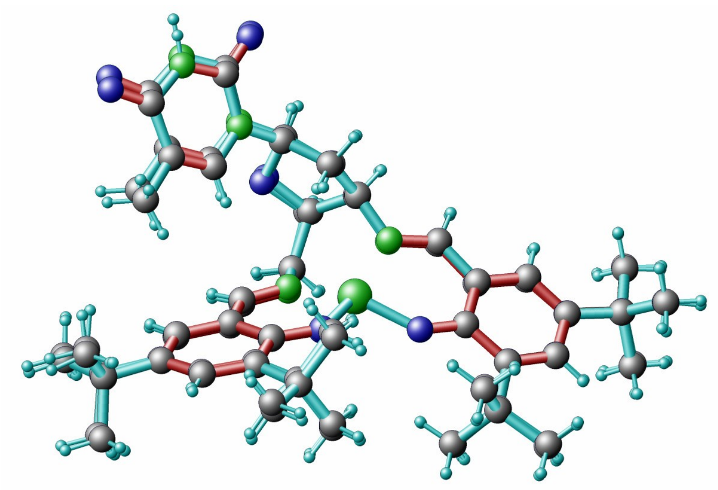
- Unknown Unknowns
  - Do we allow our specification to be incomplete?
  - Open World vs. Closed World
  - Entailment vs. Model Checking
- Known Unknowns
  - Do we allow “anonymous” elements?
  - Nulls (bnodes, existential quantifiers) vs. constants
  - No Unique Name Assumption on Nulls

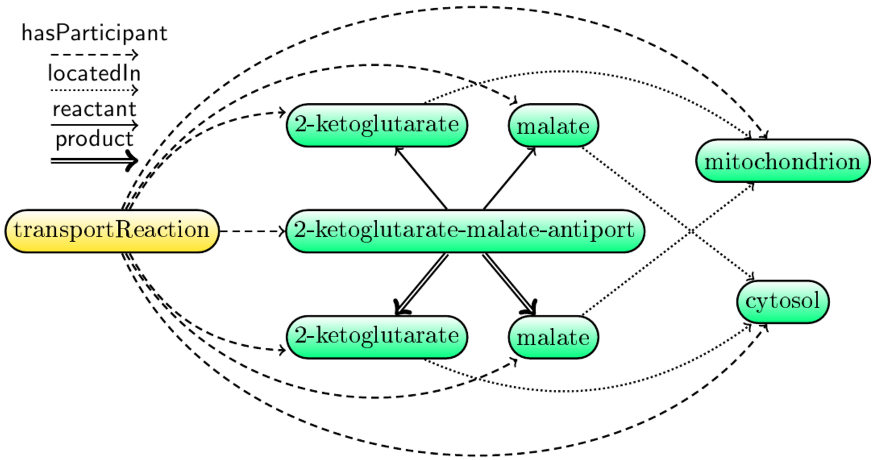
Rules and the Unknown

- Closed World & Unique Names
  - PROLOG
  - Datalog
  - …
- Open World and Anonymous Individuals:
  - Tuple Generating Dependencies
  - …

Using Rules to Model Ontologies

- Expressive advantage:
  - Rules can express complex relational structures
  - Natural compatibility with conjunctive queries
  - Well-understood non-monotonic semantics





Existential Rules

- Formulae of the form:

$$\forall \mathbf{x}.\, B1 \wedge \ldots \wedge Bn \rightarrow \exists \mathbf{y}.H1 \wedge \ldots \wedge Hk$$

  where B1, …, Bn, H1, …, Hk are logical atoms
  (we often keep the ∀ implicit)

- Also known as:
  - Tuple Generating Dependencies (TGDs)
  - Datalog+/-
  - ∀∃-rules

Reasoning with Existential Rules

- Considered as first-order logic formulae
  - Open World Semantics
  - Sometimes Unique Name Assumption on constants
- Main practical entailment problem:
  - Conjunctive query answering
- Entailment is hard:
  - Even fact entailment is undecidable in general

Existential Rules: Decidable Fragments

- Approach 1: Acyclicity
  - Limit amount of derived Nulls
  - Finite least models
- Approach 2: Guardedness
  - Limit non-local interactions in derivation
  - Tree-like least models
- Approach 3: Boundedness
  - Limit recursion to allow full expansion of rule sets
  - Rules can be rewritten to conjunctive queries

Nonmonotonic Existential Rules

- Formulae of the form:

  $\forall \mathbf{x}.\ B1 \wedge \ldots \wedge Bn \wedge \textbf{not}\ C1 \wedge \ldots \wedge \textbf{not}\ Cm \rightarrow \exists \mathbf{y}.H1 \wedge \ldots \wedge Hk$

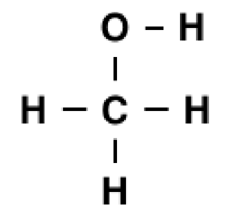
  where B1, …, Bn, C1, …, Cm, H1, …, Hk are logical atoms
  (we often keep the ∀ implicit)

- Possible Semantics of Negation:
  - Stable Model Semantics (as in ASP)
  - Well-Founded Semantics

Nonmonotonic Existential Rules: Example

[Magka, K, Horrocks: Computing Stable Models for Nonmonotonic Existential Rules. IJCAI'13]

- Modelling molecular structures with rules:



Methanol molecule

$$\mathsf{methanol}(x) \rightarrow \exists_{i=1}^{6} y_i . \bigwedge_{i=1}^{6} \mathsf{hasAtom}(x, y_i) \wedge \mathsf{c}(y_1) \wedge \mathsf{o}(y_2) \wedge \bigwedge_{i=3}^{6} \mathsf{h}(y_i) \wedge \bigwedge_{i=2}^{5} \mathsf{bond}(y_1, y_i) \wedge \mathsf{bond}(y_2, y_6)$$

- Nonmonotonic negation used to control structure:

$$\bigwedge_{i=1}^{3} \mathsf{hasAtom}(x, z_i) \wedge \ldots \wedge \mathsf{bond}(z_2, z_3) \wedge \ \mathbf{not}\ g_h(z_1) \wedge \ \mathbf{not}\ g_h(z_2) \wedge \ \mathbf{not}\ g_h(z_3) \rightarrow \mathsf{organicHydroxy}(x) \wedge r_h(x)$$

$$\mathsf{organicHydroxy}(x) \wedge \ \mathbf{not}\ r_h(x) \rightarrow \exists_{i=1}^{3} y_i . \bigwedge_{i=1}^{3} \mathsf{hasAtom}(x, y_i) \wedge \ldots \wedge \mathsf{bond}(y_2, y_3) \wedge \bigwedge_{i=1}^{3} g_h(y_i)$$

Nonmonotonic Existential Rules: Experiments

[Magka, K, Horrocks: Computing Stable Models for Nonmonotonic Existential Rules. IJCAI'13]

- Data modelled in rules:
  - 500 molecule models (from ChEBI database)
  - 30 functional groups
  - 50 chemical classes

→ 78,957 rules in total

- Query answering for classifying molecules:
  - DLV (Answer Set Solver): time out after 5min
  - Static analysis to partition rules + DLV: 13.5 sec
    → 8,639 subsumptions of chemical classes

Conclusions

- Rules can be used for ontological modelling
- Existential quantifiers to derive new structures (Nulls)
- Closed world? Open World? Mix and match!

- TODOs:
  - No unified syntax or even file format (other than RIF)
  - No tool and libraries to process and represent rules
  - No tools to model with rules
  - No reasoners optimized for ontological needs