Computing Stable Models for Nonmonotonic Existential Rules

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The OWLs are not what they seem

- OWL widely used for authoring biomedical ontologies

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GO the Gene Ontology

NCIthesaurus

BioPortal

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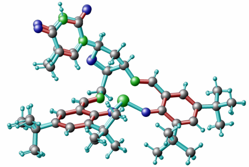

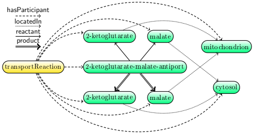

Nonmonotonic Existential Rules

- Rules with nonmonotonic negation in the body and existentials in the head

$$B_1 \wedge \ldots \wedge B_n \wedge \ \mathbf{not}\ B_{n+1} \wedge \ldots \wedge \ \mathbf{not}\ B_m \rightarrow \exists \mathbf{y}.H_1 \wedge \ldots \wedge H_k$$

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- Good for representing non-tree-shaped structures
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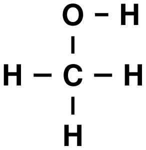
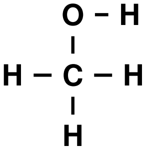
  - Nonmonotonicity adds extra expressivity in modelling
  - Stable model semantics supported by many tools: DLV, clasp, . . .

Classification of Structured Objects I



Methanol molecule

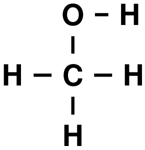
Classification of Structured Objects I



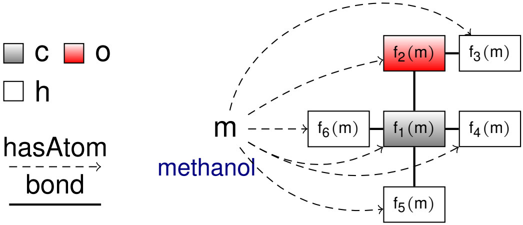
Methanol molecule

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

Classification of Structured Objects I

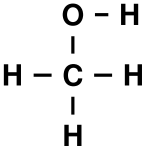


Methanol molecule

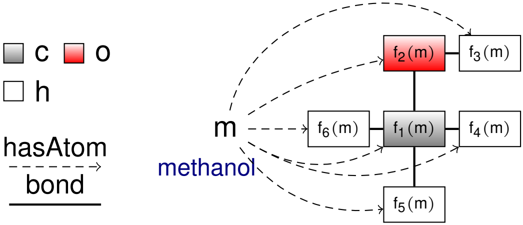


$$\text{methanol}(x) \rightarrow \exists_{i=1}^{6} y_i .\ \wedge_{i=1}^{6} \text{hasAtom}(x, y_i) \wedge c(y_1) \wedge o(y_2) \wedge \wedge_{i=3}^{6} h(y_i) \wedge \wedge_{i=2}^{5} \text{bond}(y_1, y_i) \wedge \text{bond}(y_2, y_6)$$

Classification of Structured Objects I



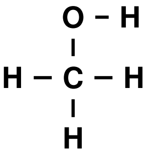
Methanol molecule



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

$$\bigwedge_{i=1}^{3} \text{hasAtom}(x, z_i) \wedge c(z_1) \wedge o(z_2) \wedge h(z_3) \wedge \text{bond}(z_1, z_2) \wedge \text{bond}(z_2, z_3) \rightarrow \text{organicHydroxy}(x)$$

Classification of Structured Objects I



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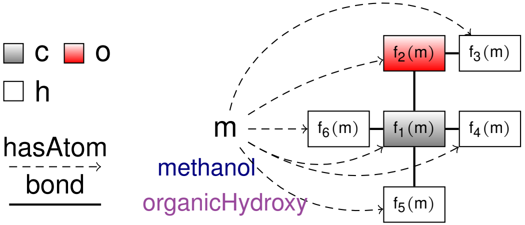
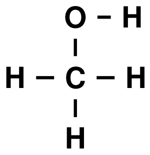


$$\text{methanol}(x) \rightarrow \exists_{i=1}^{6} y_i.\ \wedge_{i=1}^{6} \text{hasAtom}(x, y_i) \wedge c(y_1) \wedge o(y_2) \wedge$$
$$\wedge_{i=3}^{6} h(y_i) \wedge \wedge_{i=2}^{5} \text{bond}(y_1, y_i) \wedge \text{bond}(y_2, y_6)$$

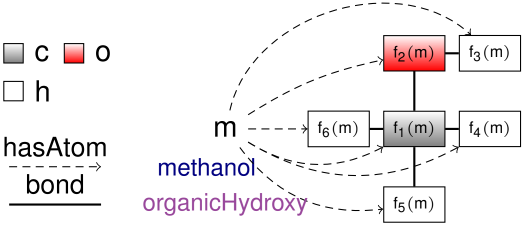
$$\wedge_{i=1}^{3} \text{hasAtom}(x, z_i) \wedge c(z_1) \wedge o(z_2) \wedge$$
$$h(z_3) \wedge \text{bond}(z_1, z_2) \wedge \text{bond}(z_2, z_3) \rightarrow \text{organicHydroxy}(x)$$

$\text{methanol} \sqsubseteq \text{organicHydroxy}$ ✓

CLASSIFICATION OF STRUCTURED OBJECTS I



Methanol molecule



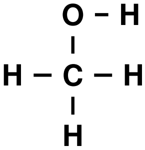
$$\text{methanol}(x) \rightarrow \exists_{i=1}^{6} y_i.\ \bigwedge_{i=1}^{6} \text{hasAtom}(x, y_i) \land c(y_1) \land o(y_2) \land \\ \bigwedge_{i=3}^{6} h(y_i) \land \bigwedge_{i=2}^{5} \text{bond}(y_1, y_i) \land \text{bond}(y_2, y_6)$$

$$\bigwedge_{i=1}^{3} \text{hasAtom}(x, z_i) \land c(z_1) \land o(z_2) \land \\ h(z_3) \land \text{bond}(z_1, z_2) \land \text{bond}(z_2, z_3) \rightarrow \text{organicHydroxy}(x)$$

$$\text{hasAtom}(x, z) \land o(z) \rightarrow \text{hasOxygen}(x)$$

$\text{methanol} \sqsubseteq \text{organicHydroxy}$ ✓

Classification of Structured Objects I



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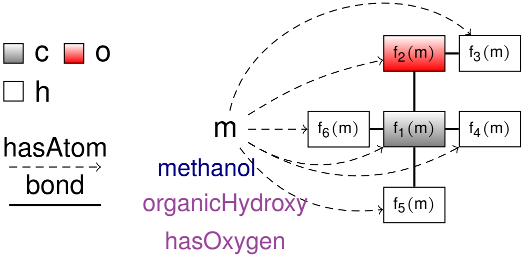


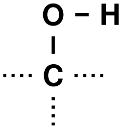
$$\mathrm{methanol}(x) \rightarrow \exists_{i=1}^{6} y_i.\ \bigwedge_{i=1}^{6} \mathrm{hasAtom}(x,y_i) \wedge c(y_1) \wedge o(y_2) \wedge \bigwedge_{i=3}^{6} h(y_i) \wedge \bigwedge_{i=2}^{5} \mathrm{bond}(y_1,y_i) \wedge \mathrm{bond}(y_2,y_6)$$

$$\bigwedge_{i=1}^{3} \mathrm{hasAtom}(x,z_i) \wedge c(z_1) \wedge o(z_2) \wedge h(z_3) \wedge \mathrm{bond}(z_1,z_2) \wedge \mathrm{bond}(z_2,z_3) \rightarrow \mathrm{organicHydroxy}(x)$$

$$\mathrm{hasAtom}(x,z) \wedge o(z) \rightarrow \mathrm{hasOxygen}(x)$$

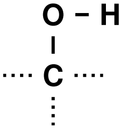
$\mathrm{methanol} \sqsubseteq \mathrm{organicHydroxy}$ ✓ $\mathrm{methanol} \sqsubseteq \mathrm{hasOxygen}$ ✓

Classification of Structured Objects II



Organic hydroxy group

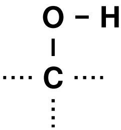
Classification of Structured Objects II



Organic hydroxy group

$$\mathsf{organicHydroxy}(x) \rightarrow \exists_{\mathsf{i}=1}^{3} \mathsf{y_i}.\ \wedge_{\mathsf{i}=1}^{3} \mathsf{hasAtom}(\mathsf{x}, \mathsf{y_i}) \wedge \mathsf{c}(\mathsf{y_1}) \\ \wedge \mathsf{o}(\mathsf{y_2}) \wedge \mathsf{h}(\mathsf{y_3}) \wedge \mathsf{bond}(\mathsf{y_1}, \mathsf{y_2}) \\ \wedge \mathsf{bond}(\mathsf{y_2}, \mathsf{y_3})$$

Classification of Structured Objects II

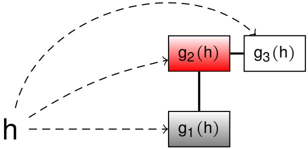


Organic hydroxy group

▨ c 🟥 o

□ h

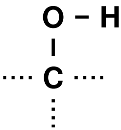
$\xrightarrow[\text{bond}]{\text{hasAtom}}$



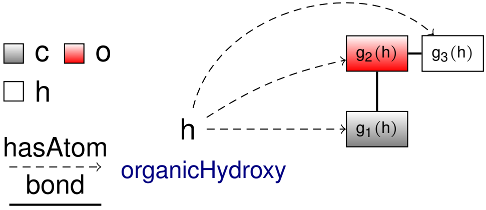
organicHydroxy

$$
\begin{aligned}
\text{organicHydroxy}(x) \rightarrow \exists_{i=1}^{3} y_i .\ \wedge_{i=1}^{3}\ &\text{hasAtom}(x, y_i) \wedge c(y_1) \\
&\wedge o(y_2) \wedge h(y_3) \wedge \text{bond}(y_1, y_2) \\
&\wedge \text{bond}(y_2, y_3)
\end{aligned}
$$

Classification of Structured Objects II



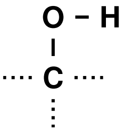
Organic hydroxy group



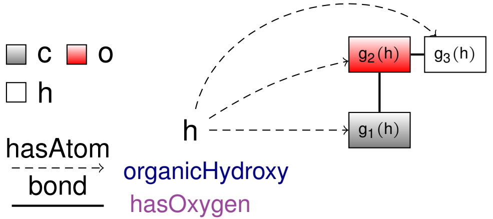
$$\text{organicHydroxy}(x) \rightarrow \exists_{i=1}^{3} y_i .\ \wedge_{i=1}^{3} \text{hasAtom}(x, y_i) \wedge c(y_1) \wedge o(y_2) \wedge h(y_3) \wedge \text{bond}(y_1, y_2) \wedge \text{bond}(y_2, y_3)$$

$$\text{hasAtom}(x, z) \wedge o(z) \rightarrow \text{hasOxygen}(x)$$

Classification of Structured Objects II



Organic hydroxy group



$$\text{organicHydroxy}(x) \rightarrow \exists^{3}_{i=1} y_i .\ \wedge^{3}_{i=1} \text{hasAtom}(x, y_i) \wedge c(y_1) \wedge o(y_2) \wedge h(y_3) \wedge \text{bond}(y_1, y_2) \wedge \text{bond}(y_2, y_3)$$

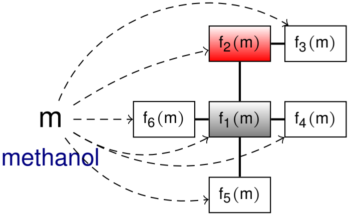
$$\text{hasAtom}(x, z) \wedge o(z) \rightarrow \text{hasOxygen}(x)$$

$$\text{organicHydroxy} \sqsubseteq \text{hasOxygen} \checkmark$$

Incorrect Modelling

$$
\begin{aligned}
\mathsf{methanol}(x) &\rightarrow \exists_{i=1}^{6} y_i .\ \wedge_{i=1}^{6} \mathsf{hasAtom}(x, y_i) \wedge \ldots \\
&\qquad\qquad \wedge\, \mathsf{bond}(y_2, y_6) \\
\wedge_{i=1}^{3} \mathsf{hasAtom}(x, z_i) \wedge \ldots \wedge & \\
\mathsf{bond}(z_2, z_3) &\rightarrow \mathsf{organicHydroxy}(x) \\
\mathsf{organicHydroxy}(x) &\rightarrow \exists_{i=1}^{3} y_i .\ \wedge_{i=1}^{3} \mathsf{hasAtom}(x, y_i) \wedge \ldots \\
&\qquad\qquad \wedge\, \mathsf{bond}(y_2, y_3) \\
\mathsf{hasAtom}(x, z) \wedge o(z) &\rightarrow \mathsf{hasOxygen}(x)
\end{aligned}
$$

Incorrect Modelling



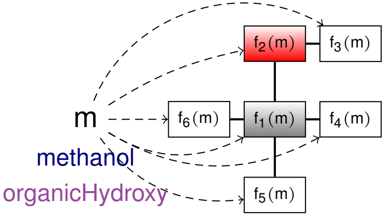
$$\mathrm{methanol}(x) \rightarrow \exists^{6}_{i=1} y_i . \bigwedge^{6}_{i=1} \mathrm{hasAtom}(x, y_i) \wedge \ldots \\ \wedge\, \mathrm{bond}(y_2, y_6)$$

$$\bigwedge^{3}_{i=1} \mathrm{hasAtom}(x, z_i) \wedge \ldots \wedge \\ \mathrm{bond}(z_2, z_3) \rightarrow \mathrm{organicHydroxy}(x)$$

$$\mathrm{organicHydroxy}(x) \rightarrow \exists^{3}_{i=1} y_i . \bigwedge^{3}_{i=1} \mathrm{hasAtom}(x, y_i) \wedge \ldots \\ \wedge\, \mathrm{bond}(y_2, y_3)$$

$$\mathrm{hasAtom}(x, z) \wedge o(z) \rightarrow \mathrm{hasOxygen}(x)$$

Incorrect Modelling



$$\text{methanol} \sqsubseteq \text{organicHydroxy} \checkmark$$

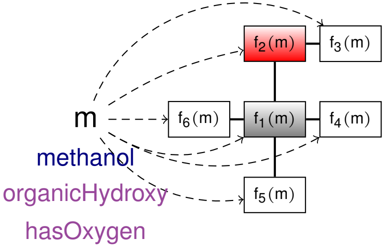
$$\text{methanol}(x) \rightarrow \exists_{i=1}^{6} y_i . \bigwedge_{i=1}^{6} \text{hasAtom}(x, y_i) \wedge \ldots \wedge \text{bond}(y_2, y_6)$$

$$\bigwedge_{i=1}^{3} \text{hasAtom}(x, z_i) \wedge \ldots \wedge \text{bond}(z_2, z_3) \rightarrow \text{organicHydroxy}(x)$$

$$\text{organicHydroxy}(x) \rightarrow \exists_{i=1}^{3} y_i . \bigwedge_{i=1}^{3} \text{hasAtom}(x, y_i) \wedge \ldots \wedge \text{bond}(y_2, y_3)$$

$$\text{hasAtom}(x, z) \wedge o(z) \rightarrow \text{hasOxygen}(x)$$

Incorrect Modelling



methanol $\sqsubseteq$ hasOxygen ✓

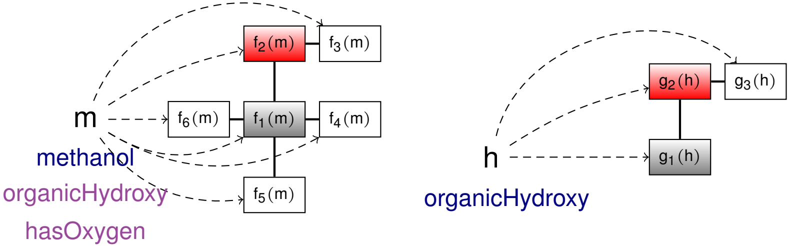
$$\mathrm{methanol}(x) \rightarrow \exists_{i=1}^{6} y_i.\ \wedge_{i=1}^{6} \mathrm{hasAtom}(x, y_i) \wedge \ldots \wedge \mathrm{bond}(y_2, y_6)$$

$$\wedge_{i=1}^{3} \mathrm{hasAtom}(x, z_i) \wedge \ldots \wedge \mathrm{bond}(z_2, z_3) \rightarrow \mathrm{organicHydroxy}(x)$$

$$\mathrm{organicHydroxy}(x) \rightarrow \exists_{i=1}^{3} y_i.\ \wedge_{i=1}^{3} \mathrm{hasAtom}(x, y_i) \wedge \ldots \wedge \mathrm{bond}(y_2, y_3)$$

$$\mathrm{hasAtom}(x, z) \wedge o(z) \rightarrow \mathrm{hasOxygen}(x)$$

Incorrect Modelling



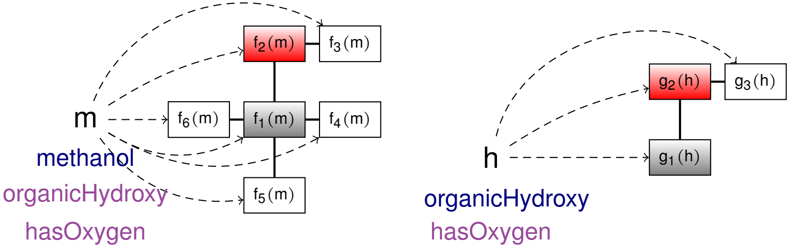
$$\text{methanol}(x) \rightarrow \exists_{i=1}^{6} y_i . \wedge_{i=1}^{6} \text{hasAtom}(x, y_i) \wedge \ldots \wedge \text{bond}(y_2, y_6)$$

$$\wedge_{i=1}^{3} \text{hasAtom}(x, z_i) \wedge \ldots \wedge \text{bond}(z_2, z_3) \rightarrow \text{organicHydroxy}(x)$$

$$\text{organicHydroxy}(x) \rightarrow \exists_{i=1}^{3} y_i . \wedge_{i=1}^{3} \text{hasAtom}(x, y_i) \wedge \ldots \wedge \text{bond}(y_2, y_3)$$

$$\text{hasAtom}(x, z) \wedge o(z) \rightarrow \text{hasOxygen}(x)$$

Incorrect Modelling



m

methanol

organicHydroxy

hasOxygen

h

organicHydroxy

hasOxygen

organicHydroxy $\sqsubseteq$ hasOxygen ✓

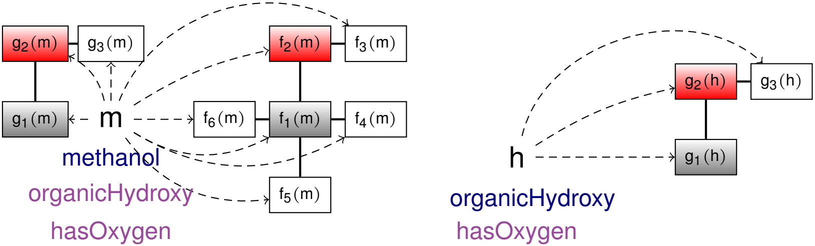
$$\text{methanol}(x) \rightarrow \exists_{i=1}^{6} y_i . \bigwedge_{i=1}^{6} \text{hasAtom}(x, y_i) \wedge \ldots \wedge \text{bond}(y_2, y_6)$$

$$\bigwedge_{i=1}^{3} \text{hasAtom}(x, z_i) \wedge \ldots \wedge \text{bond}(z_2, z_3) \rightarrow \text{organicHydroxy}(x)$$

$$\text{organicHydroxy}(x) \rightarrow \exists_{i=1}^{3} y_i . \bigwedge_{i=1}^{3} \text{hasAtom}(x, y_i) \wedge \ldots \wedge \text{bond}(y_2, y_3)$$

$$\text{hasAtom}(x, z) \wedge o(z) \rightarrow \text{hasOxygen}(x)$$

Incorrect Modelling



$$\text{methanol} \sqsubseteq \text{hasOneCarbon}$$ ✗

$$\text{methanol}(x) \rightarrow \exists^{6}_{i=1} y_i .\ \bigwedge^{6}_{i=1} \text{hasAtom}(x, y_i) \wedge \ldots \wedge \text{bond}(y_2, y_6)$$

$$\bigwedge^{3}_{i=1} \text{hasAtom}(x, z_i) \wedge \ldots \wedge \text{bond}(z_2, z_3) \rightarrow \text{organicHydroxy}(x)$$

$$\text{organicHydroxy}(x) \rightarrow \exists^{3}_{i=1} y_i .\ \bigwedge^{3}_{i=1} \text{hasAtom}(x, y_i) \wedge \ldots \wedge \text{bond}(y_2, y_3)$$

$$\text{hasAtom}(x, z) \wedge o(z) \rightarrow \text{hasOxygen}(x)$$

Repair With Auxiliary Predicates

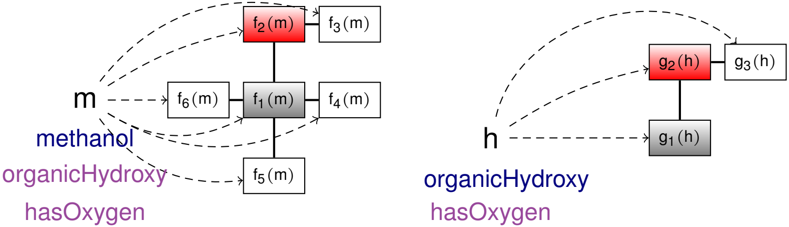
$$\mathsf{methanol}(x) \rightarrow \exists_{i=1}^{6} y_i.\ \wedge_{i=1}^{6} \mathsf{hasAtom}(x, y_i) \wedge \ldots \wedge \mathsf{bond}(y_2, y_6)$$

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

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

$$\mathsf{hasAtom}(x, z) \wedge o(z) \rightarrow \mathsf{hasOxygen}(x)$$

Repair With Auxiliary Predicates



$$\text{methanol}(x) \rightarrow \exists_{i=1}^{6} y_i.\ \wedge_{i=1}^{6}\ \text{hasAtom}(x, y_i) \wedge \ldots \wedge \text{bond}(y_2, y_6)$$

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

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$$\text{hasAtom}(x, z) \wedge o(z) \rightarrow \text{hasOxygen}(x)$$

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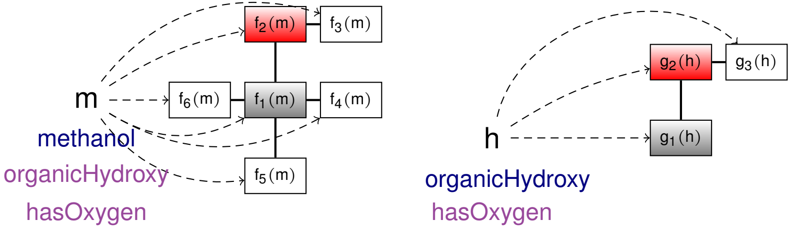

methanol
organicHydroxy
hasOxygen

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methanol $\sqsubseteq$ hasOneCarbon ✓

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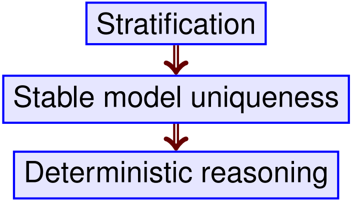

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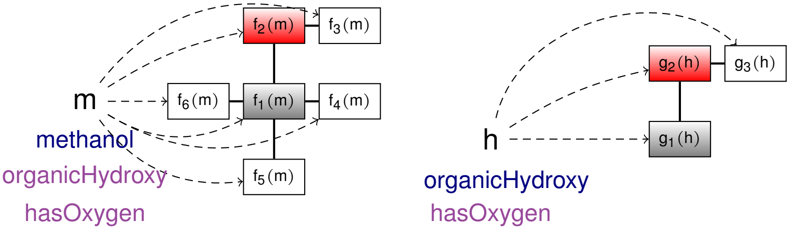

Repaired program not stratified

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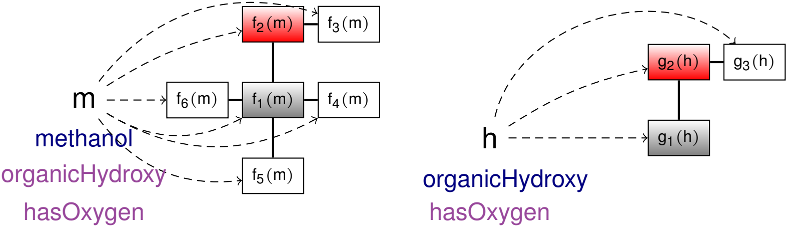

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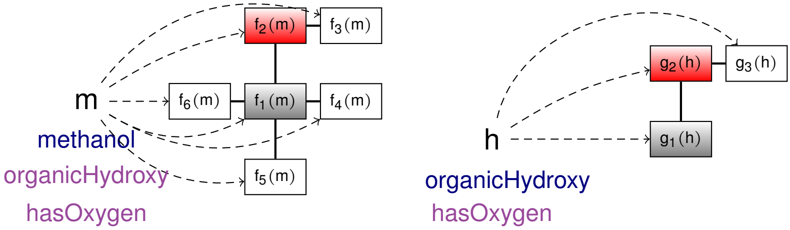

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RESULTS OVERVIEW

1. R-acyclicity and R-stratification conditions
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R-acyclic	coN2ExpTime-complete	coNP-complete
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4. Experiments over ChEBI with DLV
   - Performance gains in DLV using R-stratification
   - Missing subsumptions from ChEBI ontology

Positive reliances

- Rule r_2 positively relies on r_1 (written $r_1 \xrightarrow{+} r_2$): there is a situation when r_1 can trigger r_2 to derive something new

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Example

$$\begin{aligned} r_1 : \quad & \wedge_{i=1}^{3} \mathsf{hasAtom}(\mathsf{x}, \mathsf{z_i}) \wedge \\ & \mathsf{c}(\mathsf{z_1}) \wedge \mathsf{o}(\mathsf{z_2}) \wedge \mathsf{h}(\mathsf{z_3}) \wedge \\ & \mathsf{bond}(\mathsf{z_1}, \mathsf{z_2}) \wedge \mathsf{bond}(\mathsf{z_2}, \mathsf{z_3}) \rightarrow \mathsf{organicHydroxy}(\mathsf{x}) \end{aligned}$$

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r_2 :\quad & \boxed{\mathsf{organicHydroxy}(x)} \rightarrow \exists_{i=1}^{3} y_i . \wedge_{i=1}^{3} \mathsf{hasAtom}(x, y_i) \wedge \\
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$$r_1 \xrightarrow{+} r_2$$

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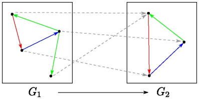

R-ACYCLICITY

- A program is R-acyclic: there is no cycle of positive reliances that involves a rule with an existential
    - Checking R-acyclicity is coNP-complete
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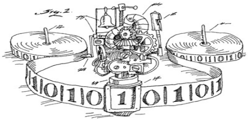

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  - coNP-complete w.r.t. data complexity

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Negative reliances

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$r_1 \overset{-}{\rightharpoonup} r_2$ but $r_2 \not\overset{-}{\rightharpoonup} r_1$

- Polynomial time to check

R-STRATIFICATION

- A program P is R-stratified if there is a partition $P_1, \ldots, P_n$ of P such that for P_i, P_j and rules $r_1 \in P_i$ and $r_2 \in P_j$, we have:

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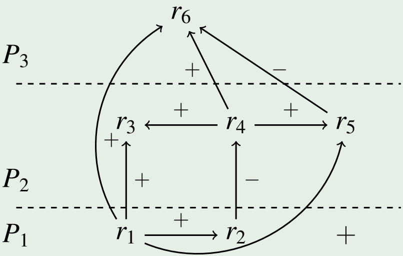

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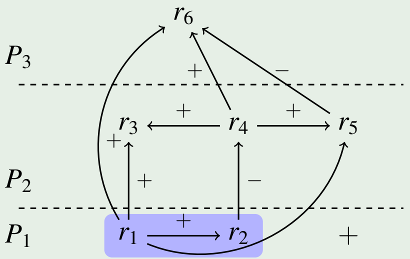

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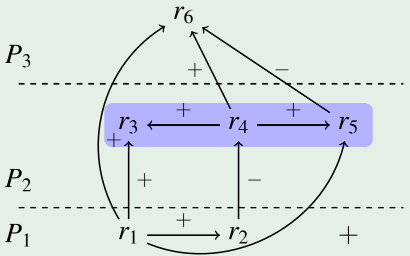

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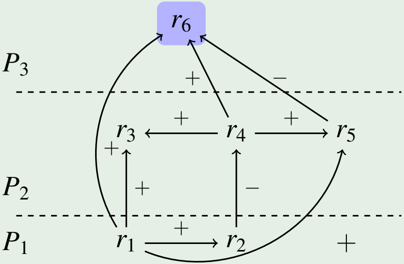

$$S^3_{\vec{\mathsf{P}}} = T_{P_3}(S^2_{\vec{\mathsf{P}}})$$

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- Restrict input sets of facts to relax R-acyclicity and R-stratification using constraints

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\begin{aligned}
r_1 :& \quad \mathsf{mol}(\mathsf{x}) \wedge \mathsf{hasAtom}(\mathsf{x}, \mathsf{z}) \wedge \mathsf{c}(\mathsf{z}) \rightarrow \mathsf{organic}(\mathsf{x}) \\
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- Slightly more complex to check:

Positive reliance	Negative reliance	R-acyclicity/R-stratification
Σ_2^P-complete	in Δ_2^P	Π_2^P-complete

$\rightsquigarrow$ Σ_2^P-hardness follows from satisfiability of a QBF $\exists\vec{p}.\forall\vec{q}.\varphi$

Experimental setup

- Chemical Entities of Biological Interest

  ChEBI
  The database and ontology of Chemical Entities of Biological Interest

  - Reference terminology adopted for chemical annotation by major bio-ontologies
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Example

$$\mathrm{methanol}(x) \rightarrow \exists_{i=1}^{6} y_i . \wedge_{i=1}^{6} \mathrm{hasAtom}(x, y_i) \wedge \ldots \wedge \mathrm{bond}(y_2, y_6)$$

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&\wedge\ \mathbf{not}\ g_h(z_2) \wedge\ \mathbf{not}\ g_h(z_3) \rightarrow \mathsf{organicHydroxy}(x) \wedge r_h(x)
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DLV

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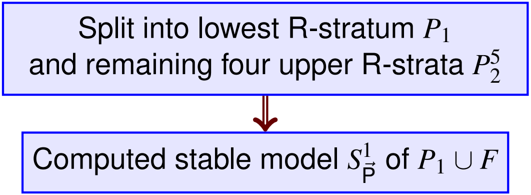

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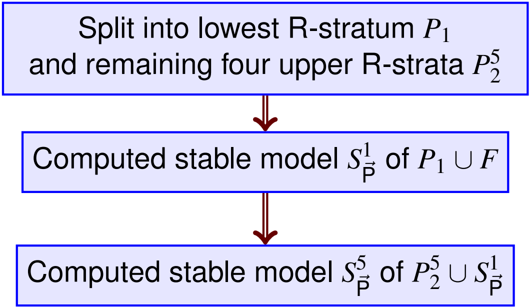

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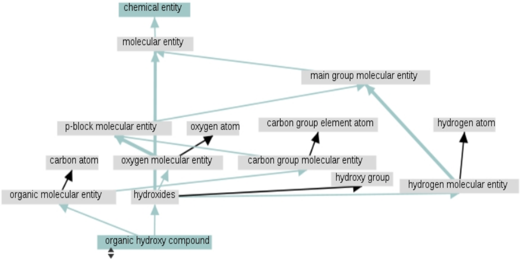
E.g. organicHydroxy $\sqsubseteq$ organoOxygenCompound ✓



✗

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