

Explanation in Ontology Languages

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With thanks to Matthew Horridge and Johannes Bauer

Outline

Mon	Introduction
Tue	Computation of justifications
Wed	Fine-grained justifications
Thu	Lemmata
Fri	Model based explanations

Monday
Introduction

Schedule for today

- Ontologies and ontology languages
- Background on explanation
- Introduction to justifications and associated services

Ontologies and ontology languages

Ontologies

- Are logical theories
- Capture a domain of interest
- Contain explicit knowledge
- Implicit knowledge can be inferred
- This is possible through the formal semantics underlying ontology languages

Ontology languages

- Often based on Description Logics (DLs)
 - Class/object/role paradigm
 - DLs have clear, formal semantics
 - (Decidable) fragments of first order logic
 - Standard, implemented inference services

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 - (Decidable) fragments of first order logic
 - Standard, implemented inference services

Many services are “automagic” (e.g., classification)

DL examples

Women are female persons.

Every mother is a female parent.

Every parent is a person.

Every parent has at least one child, each of which is a person.

DL examples

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$\text{Woman} \equiv \text{Female} \sqcap \text{Person}$

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Every mother is a female parent.

$\text{Mother} \sqsubseteq \text{Female} \sqcap \text{Parent}$

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Every parent has at least one child, each of which is a person.

$\text{Parent} \sqsubseteq \geq 1 \text{hasChild} \sqcap \forall \text{hasChild}.\text{Person}$

DL examples

Women are female persons.

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Every mother is a female parent.

$\text{Mother} \sqsubseteq \text{Female} \sqcap \text{Parent}$

Every parent is a person.

$\text{Parent} \sqsubseteq \text{Person}$

} implies:

Every mother is a woman.

$\text{Mother} \sqsubseteq \text{Woman}$

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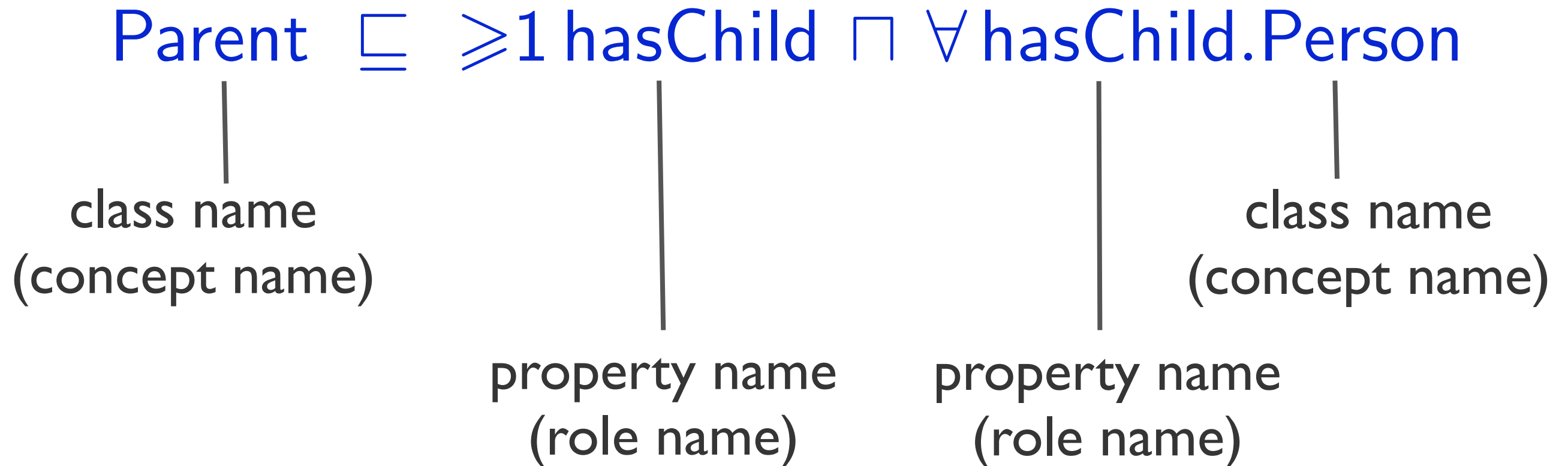
|

class name
(concept name)

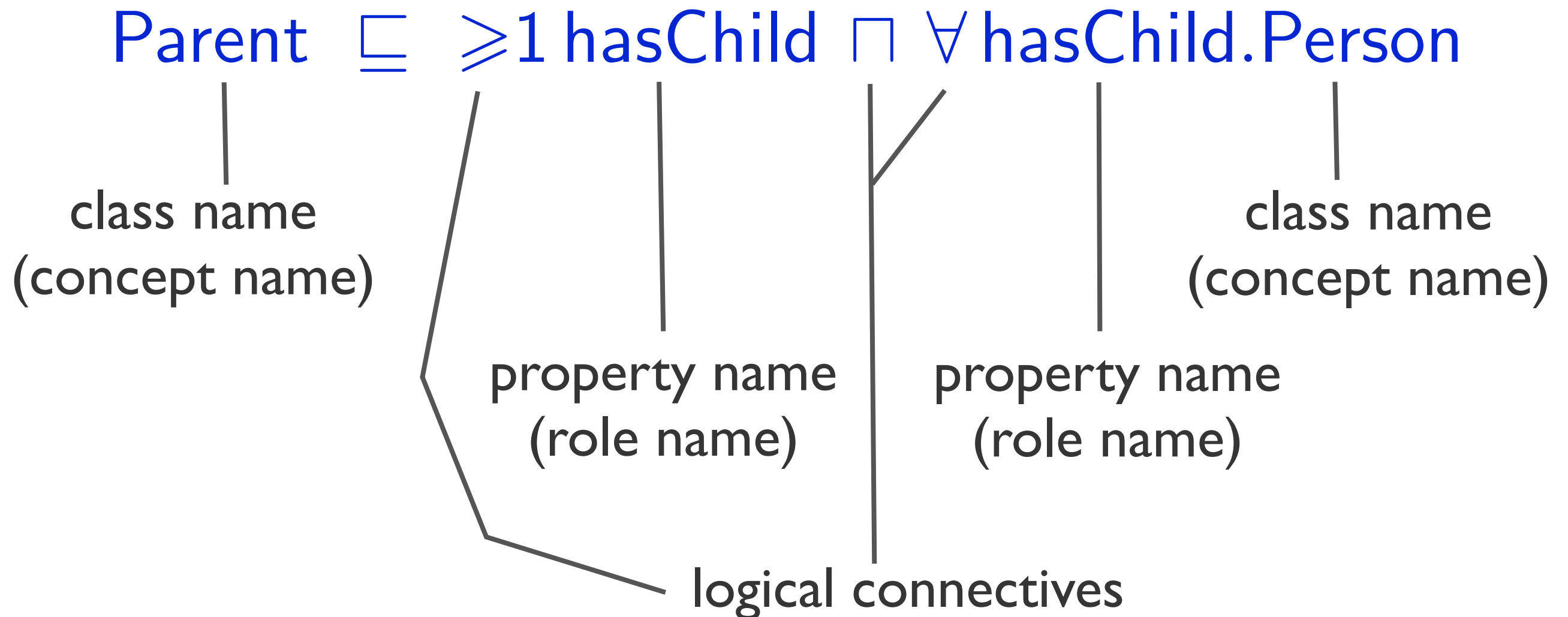
|

class name
(concept name)

DL examples



DL examples



DL examples

axiom

$\text{Parent} \sqsubseteq \geq 1 \text{ hasChild} \sqcap \forall \text{ hasChild. Person}$

class name
(concept name)

property name
(role name)

property name
(role name)

class name
(concept name)

logical connectives

DL syntax

- class names; property names:

$A, B, \dots; P, Q, \dots$

- complex classes:

$\top, A, \neg C, C \sqcap D, \exists R.C, \geq n R.C$

A atomic; C, D possibly complex;

R atomic property or inverse (P^-); $n \in \mathbb{N}$

- convention: A, B atomic classes; C, D, \dots arbitrary
- syntactic sugar:

$$\perp = \neg \top$$

$$\forall R.C = \neg \exists R. \neg C$$

$$C \sqcup D = \neg C \sqcap \neg D$$

$$\leq n R.C = \neg (\geq n+1 R.C)$$

DL syntax

$C \sqsubseteq D$ subClassOf axiom

$C \equiv D$ shortcut for $C \sqsubseteq D$ and $D \sqsubseteq C$

$R_1 \circ \dots \circ R_n \sqsubseteq S$ subPropertyChain axiom

+ more features, mostly syntactic sugar:
disjointness, transitivity, reflexivity, ...

DL syntax vs. OWL Manchester syntax

DL

concept, role

\top, \perp

$\neg C$

$C \sqcap D, C \sqcup D$

$\exists R.C, \forall R.C$

$\geq n R.C, \leq n R.C$

$=n R.C$

OWL Manchester syntax

class, property

Thing, Nothing

not C

C and D , C or D

R some C , R only C

R min $n C$, R max $n C$

R exactly $n C$

DL semantics

- Interpretations $\mathcal{I} = (\Delta^{\mathcal{I}}, \cdot^{\mathcal{I}})$ $\Delta^{\mathcal{I}} \neq \emptyset!$
with $A^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}}$ for class names A
and $P^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}} \times \Delta^{\mathcal{I}}$ for property names P

- Inductive transfer to arbitrary props / classes

$$(P^{-})^{\mathcal{I}} = \{(x, y) \mid (y, x) \in P^{\mathcal{I}}\}$$

$$\top^{\mathcal{I}} = \Delta^{\mathcal{I}}$$

$$(\neg C)^{\mathcal{I}} = \Delta^{\mathcal{I}} \setminus C^{\mathcal{I}}$$

$$(C \sqcap D)^{\mathcal{I}} = C^{\mathcal{I}} \cap D^{\mathcal{I}}$$

$$(\exists R.C)^{\mathcal{I}} = \{x \in \Delta^{\mathcal{I}} \mid \text{for some } y \in C^{\mathcal{I}}, (x, y) \in R^{\mathcal{I}}\}$$

$$(\geq n R.C)^{\mathcal{I}} = \{x \in \Delta^{\mathcal{I}} \mid \#\{y \in C^{\mathcal{I}} \mid (x, y) \in R^{\mathcal{I}}\} \geq n\}$$

DL semantics

Interpretation \mathcal{I} satisfies ...

- axiom $A \sqsubseteq B$ if $A^{\mathcal{I}} \subseteq B^{\mathcal{I}}$
- axiom $R_1 \circ \dots \circ R_n \sqsubseteq S$ if:
whenever $xR_1^{\mathcal{I}}z_1R_2^{\mathcal{I}}z_2R_3^{\mathcal{I}} \dots R_{n-1}^{\mathcal{I}}z_{n-1}R_n^{\mathcal{I}}y$,
then $xS^{\mathcal{I}}y$

We write $\mathcal{I} \models \alpha$.

We write $\mathcal{I} \models \mathcal{O}$ if $\mathcal{I} \models \alpha$ for all $\alpha \in \mathcal{O}$.

DL semantics

- Interpretation \mathcal{I} is a *model* of ontology \mathcal{O} if \mathcal{I} satisfies every axiom in \mathcal{O} .

We write $\mathcal{I} \models \mathcal{O}$.

- Ontology \mathcal{O} is *inconsistent* if it has no model.
- Class C is *satisfiable* if $C^{\mathcal{I}} \neq \emptyset$ for every interpretation \mathcal{I} .
- Axiom α is *entailed* by \mathcal{O} ($\mathcal{O} \models \alpha$) if for all \mathcal{I} : $\mathcal{I} \models \mathcal{O} \Rightarrow \mathcal{I} \models \alpha$

Ontologies

(Bio-)Medicine

Chemistry

Astronautics

... are used
in these fields
and others

Linguistics

Description of
business processes

(Web) Service
description

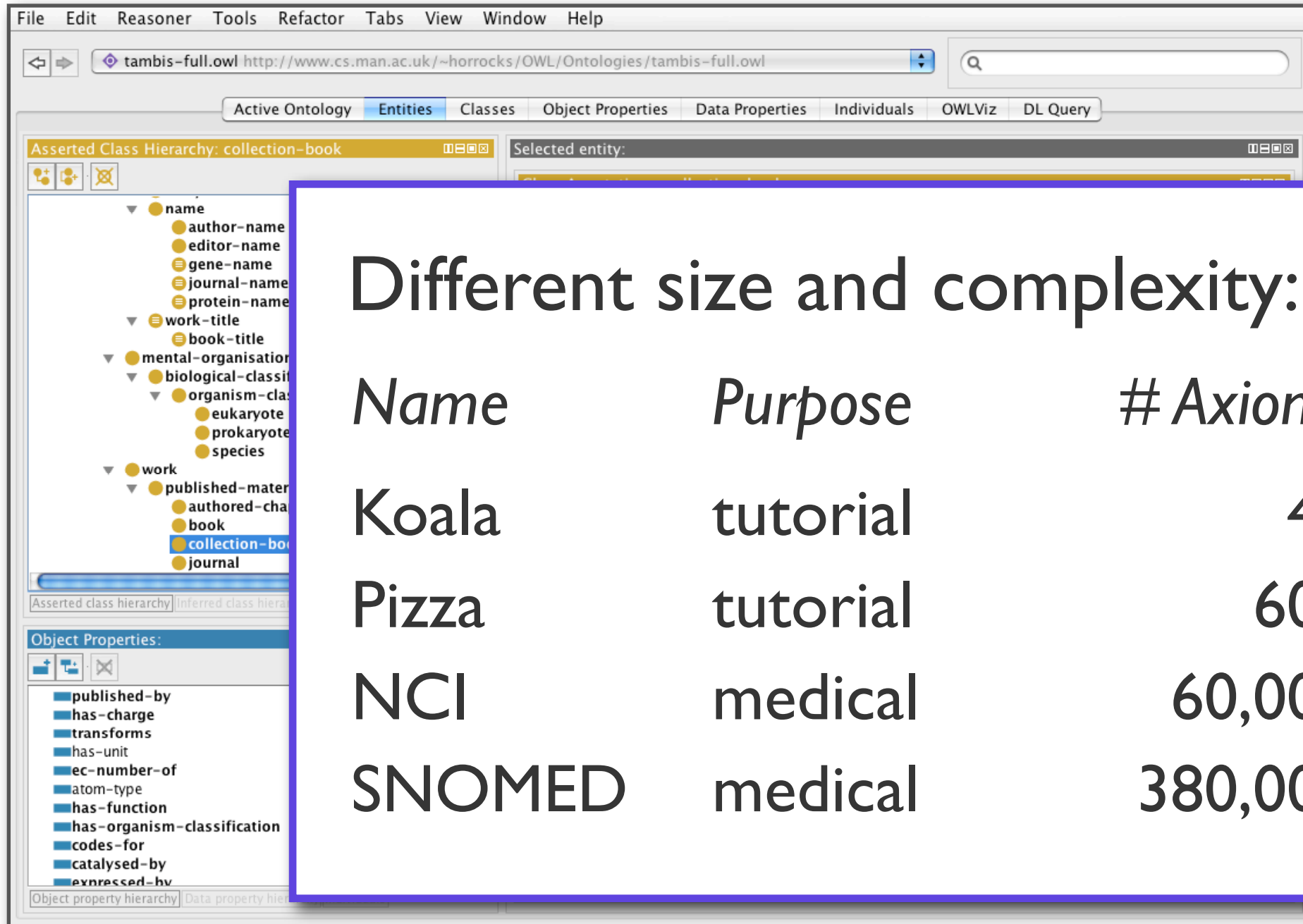
Ontologies

The screenshot displays the Protégé ontology editor interface. The top menu bar includes File, Edit, Reasoner, Tools, Refactor, Tabs, View, Window, and Help. The address bar shows the file path: `tambis-full.owl` with the URL `http://www.cs.man.ac.uk/~horrocks/OWL/Ontologies/tambis-full.owl`. The main interface is divided into several panes:

- Active Ontology:** Includes tabs for Entities, Classes, Object Properties, Data Properties, Individuals, OWLViz, and DL Query. The 'Entities' tab is currently active.
- Asserted Class Hierarchy: collection-book:** A tree view showing the hierarchy of classes. The 'collection-book' class is highlighted. Its hierarchy includes:
 - name
 - author-name
 - editor-name
 - gene-name
 - journal-name
 - protein-name
 - work-title
 - book-title
 - mental-organisation
 - biological-classification
 - organism-classification
 - eukaryote
 - prokaryote
 - species
 - work
 - published-material
 - authored-chapter
 - book
 - collection-book (highlighted)
 - journal

- Object Properties:** A list of object properties including published-by, has-charge, transforms, has-unit, ec-number-of, atom-type, has-function, has-organism-classification, codes-for, catalysed-by, and expressed-by.
- Selected entity: collection-book:** A pane showing the selected entity's details.
- Class Annotations: collection-book:** A section for class annotations.
- Class Description: collection-book:** A section showing the class description, including:
 - Equivalent classes: +
 - Superclasses: +
 - published-material
 - has-editor some editor-name
 - has-part some authored-chapter
 - has-part min 1 Thing
 - Inherited anonymous classes:
 - published-by some publishing-institution
 - has-title some work-title
 - has-publication-year some year
 - published-by only publishing-institution
 - structure and mental
 - Instances: +

Ontologies



The screenshot shows the Protégé ontology editor interface. The 'Entities' tab is active, displaying the 'Asserted Class Hierarchy: collection-book'. The hierarchy includes classes like 'name', 'author-name', 'editor-name', 'gene-name', 'journal-name', 'protein-name', 'work-title', 'book-title', 'mental-organisation', 'biological-classification', 'organism-classification', 'eukaryote', 'prokaryote', 'species', 'work', 'published-material', 'authored-chapter', 'book', 'collection-book', and 'journal'. The 'Object Properties' panel at the bottom lists properties such as 'published-by', 'has-charge', 'transforms', 'has-unit', 'ec-number-of', 'atom-type', 'has-function', 'has-organism-classification', 'codes-for', 'catalysed-by', and 'expressed-by'.

Different size and complexity:

<i>Name</i>	<i>Purpose</i>	<i># Axioms</i>
Koala	tutorial	45
Pizza	tutorial	600
NCI	medical	60,000
SNOMED	medical	380,000

Ontologies

SWOOP v2.3 beta 3.1 (Jan 2006)

File View Bookmarks Resource Holder Advanced About

Address: <http://miniTambis>

Ontology List: miniTambis

Buttons: Add Add Add Add GCI Remove Rename

Options: ☒ Show Imports ☐ QNames No Reasoner

Class Tree Property Tree List

- Binding
- binding-site
- BindingSite
 - ChemicalBindingSite
- biological-classification
 - organism-classification
 - prokaryote
- biological-function
 - obsolete
 - protein-tagging
 - regulation
 - ribosomal-rna-function
 - signal-transduction
 - receptor
 - receptor-signalling-protein
 - small-nuclear-rna-function
 - small-nucleolar-rna-function
- carbohydrate
- carbon

Lookup ☐ All Ontologies?

Ontology Info Species Validation

OWL Ontology: [miniTambis](#)

Annotations:

Total Number of Classes: 184 (Defined: 184, Imported: 0)
 Total Number of Datatype Properties: 0 (Defined: 0, Imported: 0)
 Total Number of Object Properties: 44 (Defined: 44, Imported: 0)
 Total Number of Annotation Properties: 0 (Defined: 0, Imported: 0)
 Total Number of Individuals: 0 (Defined: 0, Imported: 0)

Advanced Ontology Statistics:

General Statistics	Property Tree Statistics	Satisfiable Class Tree Statistics
DL Expressivity: ALCF No. of GCI's: 0 No. of Sub-classes: 69 No. of Disjoint Axioms: 3 No. of Functional Properties: 0 No. of Inverse Functional Properties: 0 No. of Transitive Properties: 0 No. of Symmetric Properties: 0 No. of Inverse Properties: 0	Properties with Multiple Inheritance: 0 Max. Depth of Property Tree: 2 Min. Depth of Property Tree: 2 Avg. Depth of Property Tree: ?	Classes with Multiple Inheritance: 0 Max. Depth of Class Tree: 5 Min. Depth of Class Tree: 1 Avg. Depth of Class Tree: 1.5 Max. Branching Factor of Class Tree: 110 Min. Branching Factor of Class Tree: 1 Avg. Branching Factor of Class Tree: 3.6

Ontologies




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Ontology List

miniTambis

Add  Add  Add 

Add GCI Remove Rename

☒ Show Imports ☐ QNames No Reasoner




Class Tree Property Tree List

Class Tree

- Binding
- binding-site
- BindingSite
 - ChemicalBindingSite
- biological-classification
 - organism-classification
 - prokaryote
- biological-function
 - obsolete
 - protein-tagging
 - regulation
 - ribosomal-rna-function
 - signal-transduction
 - receptor
 - receptor-signalling-protein
 - small-nuclear-rna-function
 - small-nucleolar-rna-function
- carbohydrate
- carbon

Lookup ☐ All Ontologies?

OWL Ontology Annotation

Add  Add  Add 

Add GCI Remove Rename

☒ Show Imports ☐ QNames Pellet

Class Tree Property Tree List

Class Tree

- substance
- xsd:integer

Advanced

General Statistics	Property Tree Statistics	Satisfiable Class Tree Statistics
DL Expressivity: ALCF No. of GCIs: 0 No. of Sub-classes: 69 No. of Disjoint Axioms: 3 No. of Functional Properties: 0 No. of Inverse Functional Properties: 0 No. of Transitive Properties: 0 No. of Symmetric Properties: 0 No. of Inverse Properties: 0	Properties with Multiple Inheritance: 0 Max. Depth of Property Tree: 2 Min. Depth of Property Tree: 2 Avg. Depth of Property Tree: ?	Classes with Multiple Inheritance: 0 Max. Depth of Class Tree: 5 Min. Depth of Class Tree: 1 Avg. Depth of Class Tree: 1.5 Max. Branching Factor of Class Tree: 110 Min. Branching Factor of Class Tree: 1 Avg. Branching Factor of Class Tree: 3.6

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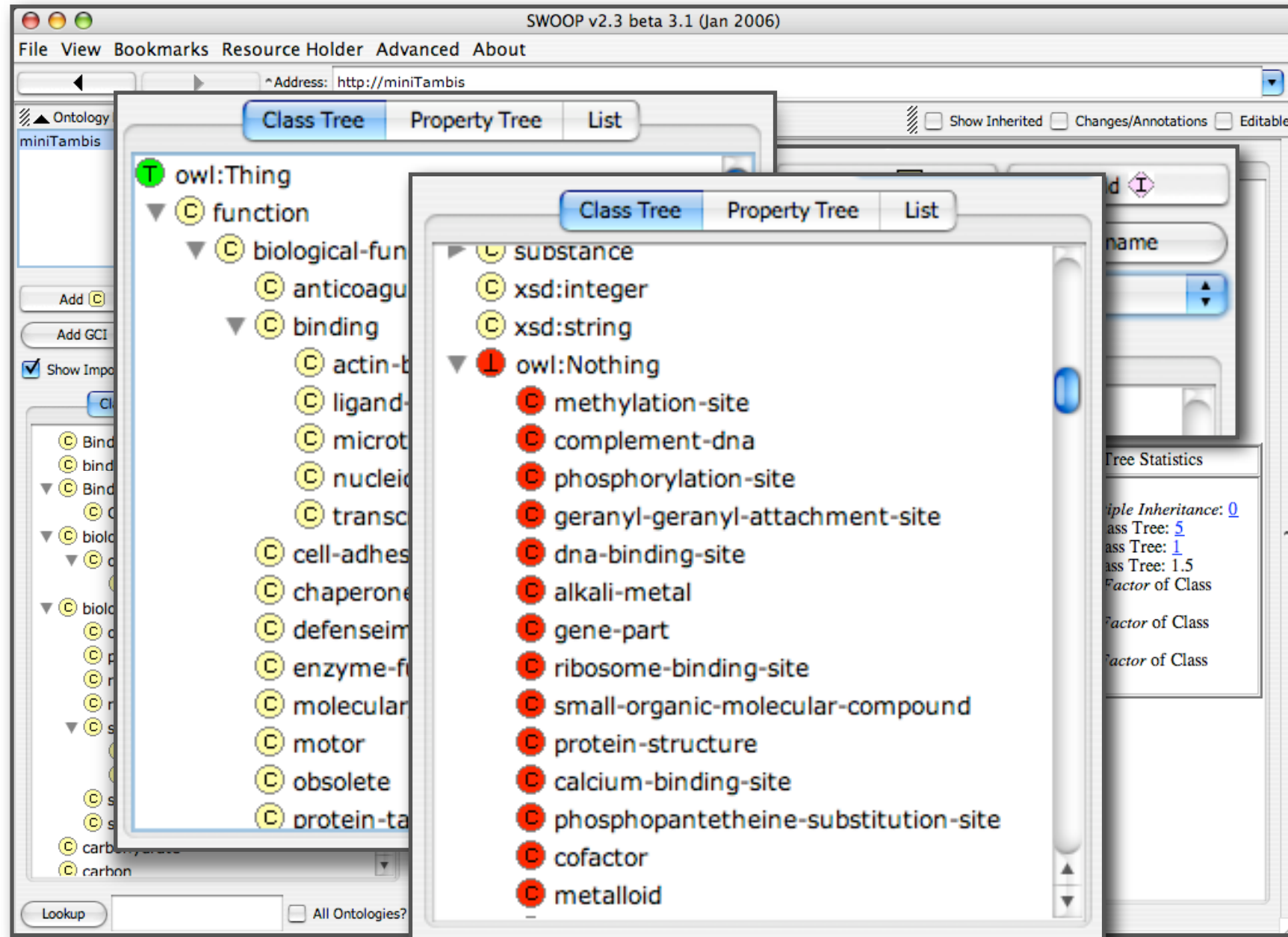
Class Tree Property Tree List

owl:Thing

- function
 - biological-function
 - anticoagulant
 - binding
 - actin-binding
 - ligand-binding-or-carrier
 - microtubule-binding
 - nucleic-acid-binding
 - transcription-factor-binding
- cell-adhesion
- chaperone
- defenseimmunity-protein
- enzyme-function
- molecular_function-unknown
- motor
- obsolete
- protein-tagging

Tree Statistics

Tree Statistics	Satisfiable Class Tree Statistics
Classes with Multiple Inheritance: 0	Classes with Multiple Inheritance: 0
Max. Depth of Class Tree: 5	Max. Depth of Class Tree: 5
Min. Depth of Class Tree: 1	Min. Depth of Class Tree: 1
Avg. Depth of Class Tree: 1.5	Avg. Depth of Class Tree: 1.5
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“Large” User Base

- Large and Growing
 - (126,870 registered Protégé Users)
 - (Standardization helps)
 - Bio-medical applications huge
- Useful for research!
 - Diverse users, tasks, issues
 - High impact

Reasoning services

Name

Question

Consistency checking

$$\mathcal{O} \models \top \sqsubseteq \perp ?$$

Subsumption checking

$$\mathcal{O} \models C \sqsubseteq D ?$$

Class hierarchy computation

$$\mathcal{O} \models A \sqsubseteq B ?$$

Unsatisfiability test

$$\mathcal{O} \models C \sqsubseteq \perp ?$$

Instance checking

$$\mathcal{O} \models a : C ?$$

Reasoning services ...

- ... are interreducible, e.g.:

$$\begin{array}{ll} \mathcal{O} \models T \sqsubseteq \perp & \iff \mathcal{O} \models A \sqcup \neg A \sqsubseteq \perp \\ \mathcal{O} \models C \sqsubseteq D & \iff \mathcal{O} \models C \sqcap \neg D \sqsubseteq \perp \end{array}$$

~> Let's focus on unsatisfiability!

- ... do not provide explanations

Need for explanations


- Some entailments undesirable (e.g., unsatisfiable classes)
- Debugging necessary
~> delete/repair axioms responsible,
but which axioms?
- Needle(s) in the haystack (of a large ontology)

Background on explanation

Context!

	Time	
	Development	Deployment
Ontology Developer		
App Programmer		
App user		

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OntEng Tasks

Understanding entailments

Debugging and repair

Understanding justifications

Ontology comprehension

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Understanding entailments

Debugging and repair

Understanding justifications

Ontology comprehension

Understanding entailments

- User notices an entailment.
- Decides to obtain an explanation for it in order to find out why it holds.

Understanding justifications

- Justification for an entailment in an ontology has been obtained.
- User wants to understand the justification better.

Ontology comprehension

- User is faced with a new ontology.
- Wants to get a better picture of it.
- Among the possible metrics:
 - ➔ Number of entailments
 - ➔ Average number of justifications for an entailment
 - ➔ ...

Debugging and repair

- User is faced with
 1. an inconsistent ontology
 2. an unsatisfiable class
 3. or “some” undesired entailment.
- Determine the cause and debug.

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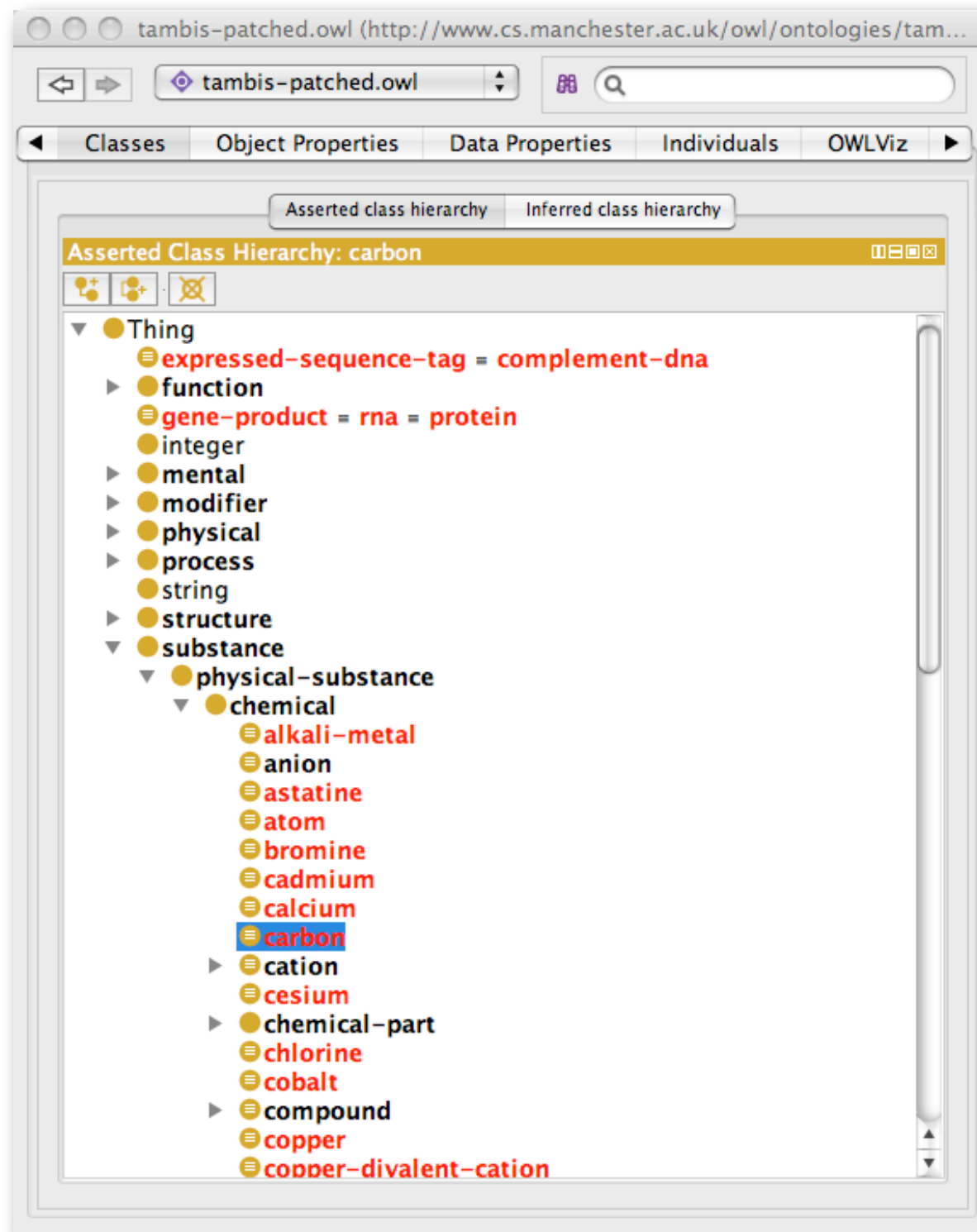
1 & 2 have high,
visible user value

Manual Debugging

Life without explanations

- Open and classify the TAMBIS ontology [tambis-patched.owl](#) in Protégé
- Open the “Asserted class hierarchy” and expand the following terms:
 - substance
 - physical-substance
 - chemical

Life without explanations



Oops!

144 out of 395 classes
are unsatisfiable (**red**).

Why?

Why are my classes unsatisfiable?

- What have we said in the ontology that **causes** these classes to be unsat?
- What do we have to change to **repair** it?
- Where do we **start**?

Where do we start? Tracing

- Open and classify the TAMBIS ontology [tambis-patched.owl](#) in Protégé
- Open the “Asserted class hierarchy” and expand the following terms:

substance

physical-substance

chemical

organic-molecular-compound

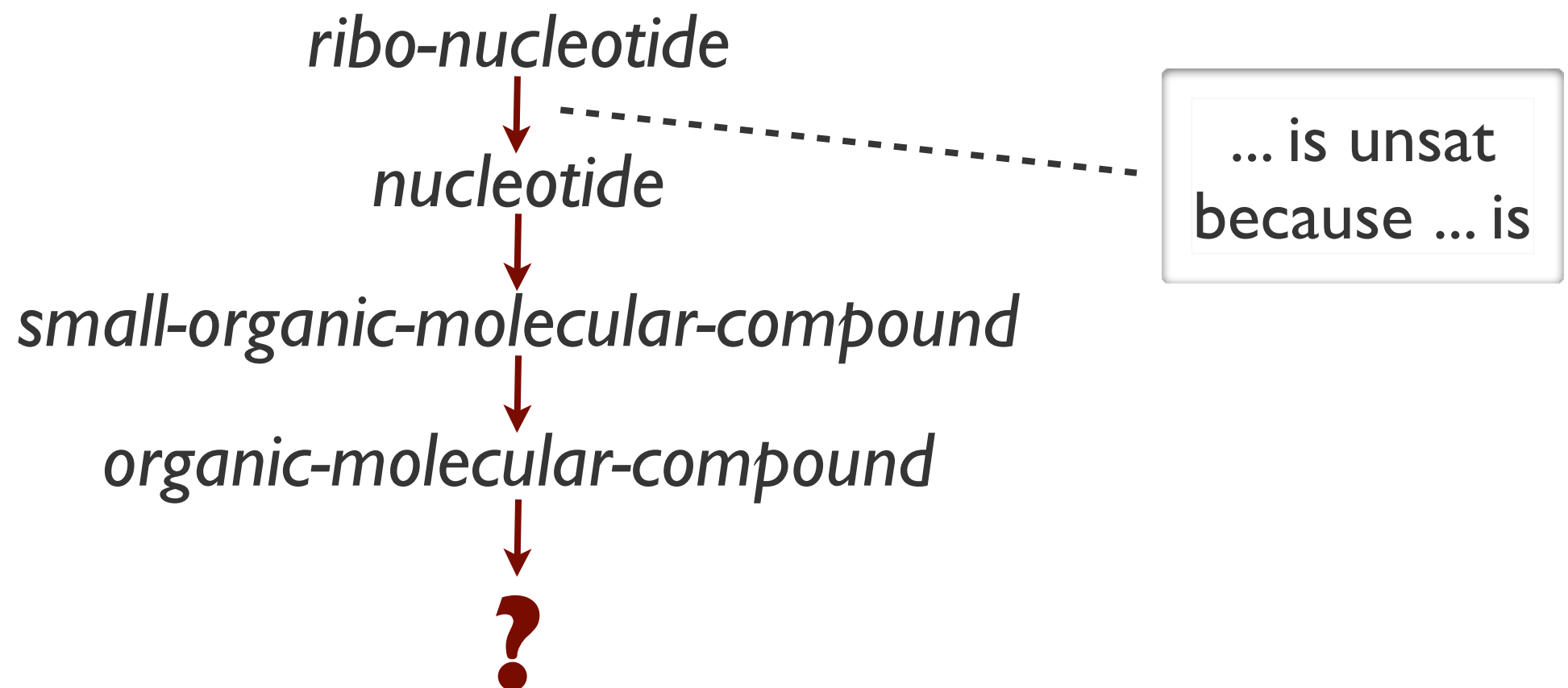
small-organic-molecular-compound

nucleotide

ribo-nucleotide

Where do we start? Tracing

Navigate through the subclass hierarchy.
If a class is unsat, then so are its subclasses.



Tracing in the old days

The only way was to manually follow ...

- unsatisfiable named superclasses
- or unsatisfiable fillers of restrictions in anonymous superclasses:

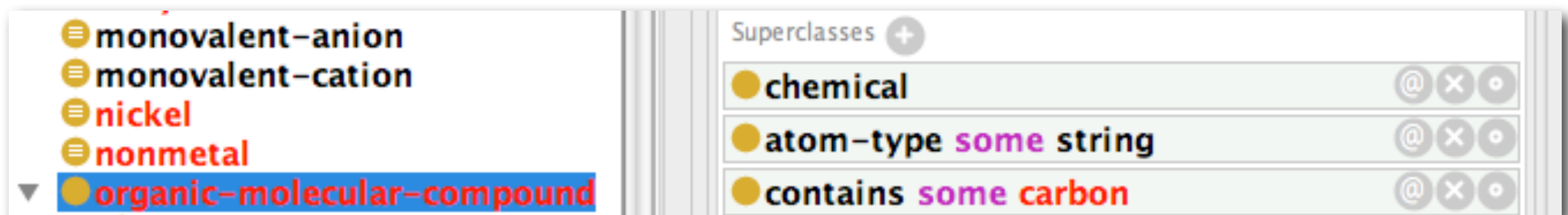
The screenshot shows a knowledge base interface. On the left, a list of classes is displayed with expandable icons (three horizontal lines). The classes are: monovalent-anion, monovalent-cation, nickel, nonmetal, and organic-molecular-compound. The 'organic-molecular-compound' class is highlighted with a blue background. On the right, a 'Superclasses' panel is visible, containing a list of superclasses: chemical, atom-type some string, and contains some carbon. Each superclass entry has a yellow circle icon, a text label, and three control buttons (a circle with '@', a circle with 'X', and a circle with a dot). A red arrow originates from the 'organic-molecular-compound' class in the left panel and points to the 'contains some carbon' restriction in the 'Superclasses' panel.

Class	Superclasses
monovalent-anion	
monovalent-cation	
nickel	
nonmetal	
organic-molecular-compound	chemical atom-type some string contains some carbon

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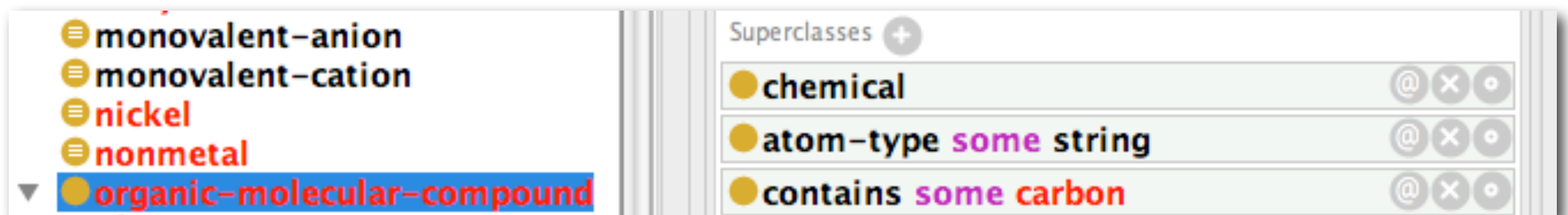


Tedious for big ontologies! ☹️

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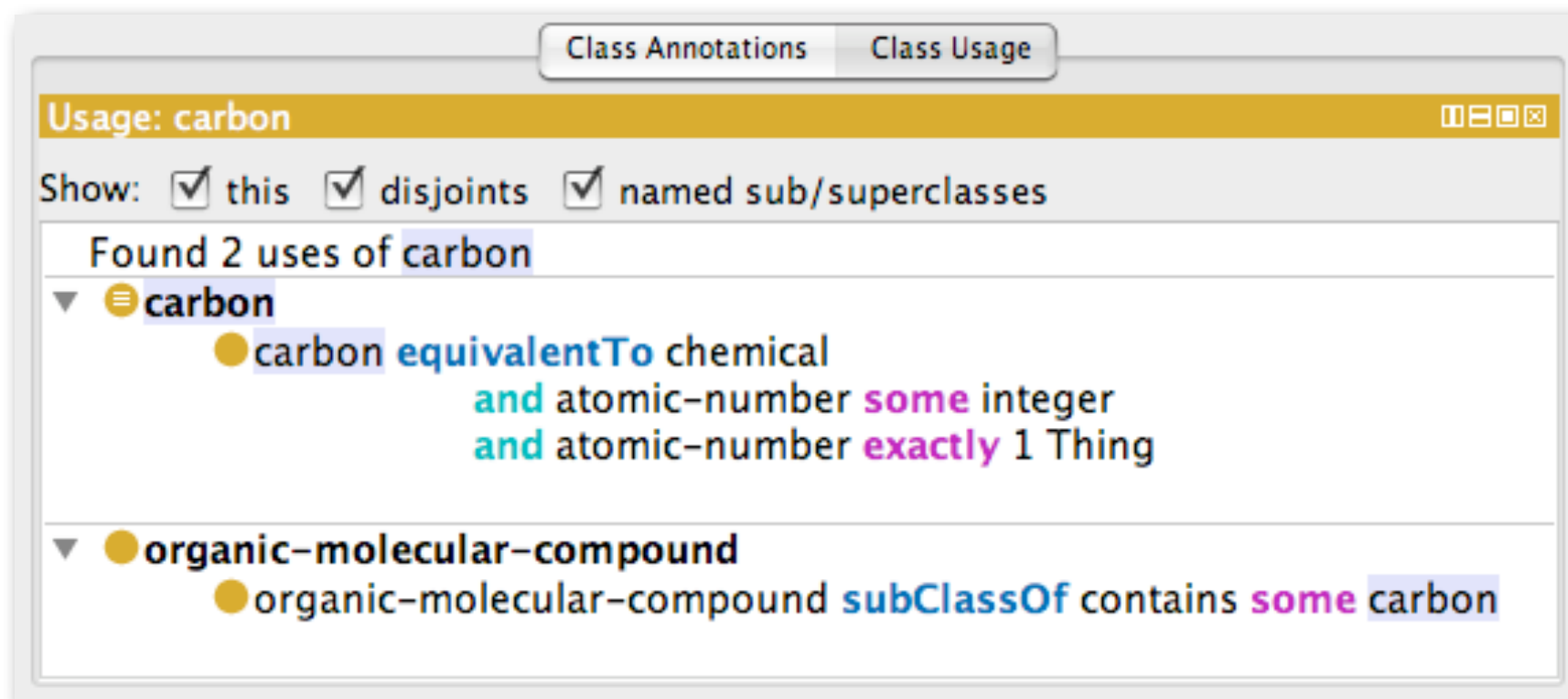


Tedious for big ontologies! 😞
May have comprehension benefits! 😊

Tracing in the old days

Now why is the root *carbon* unsatisfiable?

- Axioms may be spread throughout the ontology.
- Reasons for unsat may be highly non-obvious.



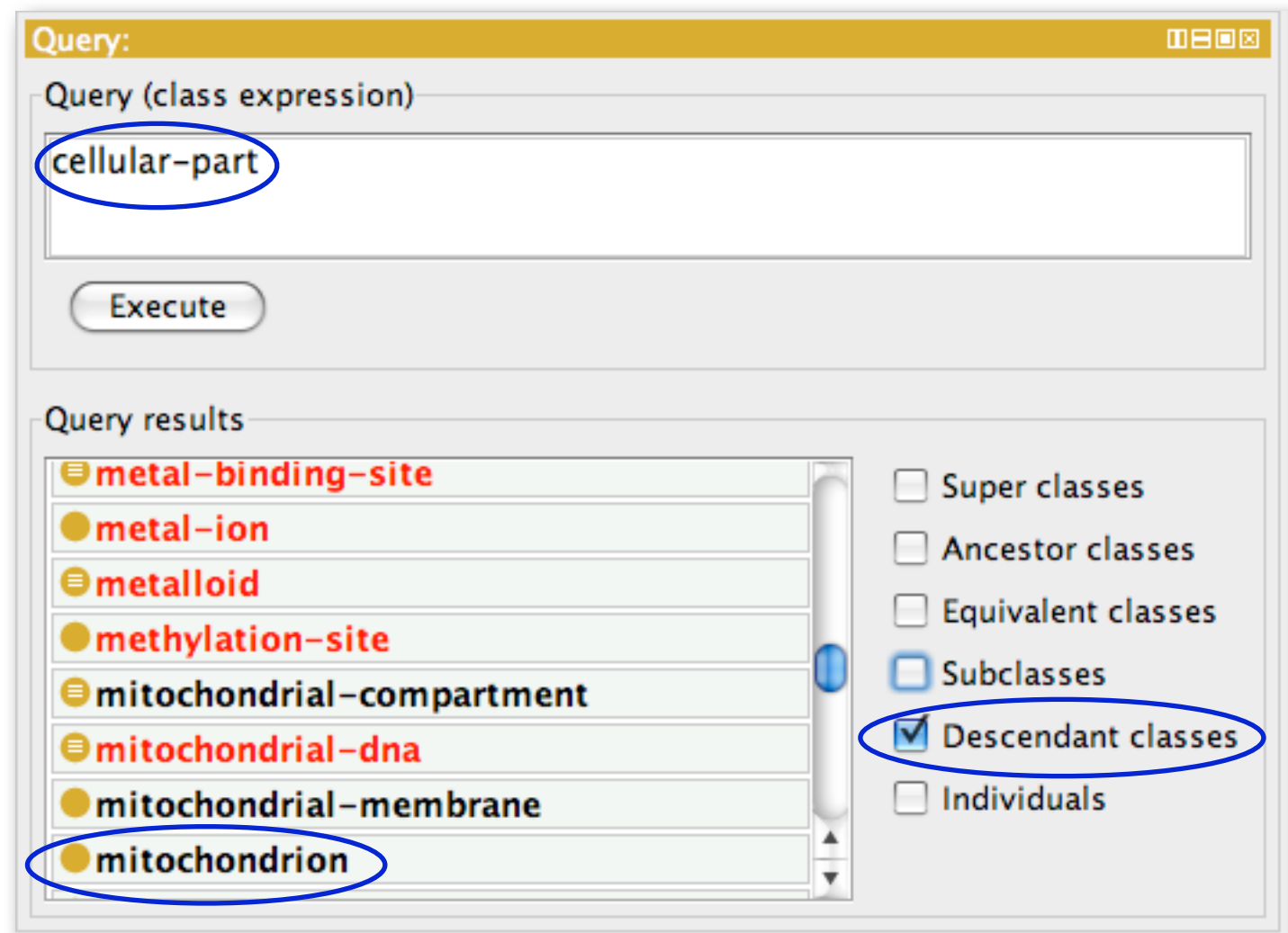
Other entailments

What about inferred subsumptions between two class names?

mitochondrion



cellular-part



Tracing difficult and not obvious

Tracing Issues

- Identifies problem **classes**/terms
 - Not problem **axioms**
- Not all problem axioms “stick” with terms
 - Tracing can’t find these
 - Depends on **definition view** of tool
 - **Binary search** of ontology?
- **Multiple** problem classes
 - **Multiple** sets of problem axioms

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Navigational approaches insufficient

Explanation

- Reasons for entailments are often difficult to understand. ~> Tool support is required.
- Theoretical basis of explanation has been investigated. New services have been defined.
- Tool support has gone from *None* to *Respectable*.
- It's now fairly easy to get explanations.
With focus: **Justifications**