Ontology engineering with rough concepts and vague instances

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Motivations

- Extending the TOG [Kee08] with roughness
- Hypothesis testing with bio-ontologies linked to data [KRM07]:
  - *Which bacteria are promiscuous?*
  - *Which properties are necessary or sufficient to identify and retrieve promiscuous bacteria?*
- DL & vagueness: fuzzy or rough
  - Based on the chosen properties, some instances are *indistinguishable*
  - Do not deal with degree of membership, but with *definitely* or *possibly* being a promiscuous bacterium
  - Hence, roughness
- What about using notions of rough sets at the knowledge representation layer?

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- Related works [BS09, FDEL08, IGNI07, JWTX09, Lia96, SKP07]:
  - Diverge in commitment as to which aspects of rough sets are included in the ontology language
  - Theory instead of demonstrating successful use of the rough DL in applications and ontology engineering
- What are the requirements for rough DL knowledge bases to faithfully *represent* the core notions of rough sets and to *implement* it?

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  - Theory instead of demonstrating successful use of the rough DL in applications and ontology engineering
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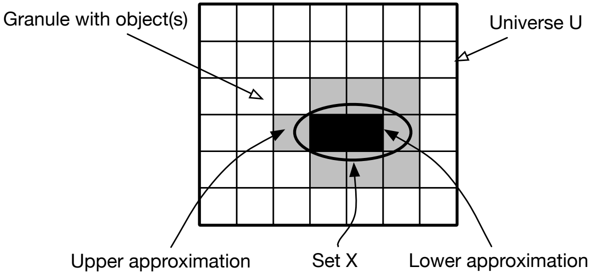
Pawlak rough set model



Pawlak rough set model

- $I = (U, A)$ is called an information system, U universe of objects
- A set of attributes s.t. for every $a \in A$, $a : U \mapsto V_a$, with V_a the set of values that attribute a can have
- For any subset of attributes $P \subseteq A$, one defines the indistinguishability relation $\text{IND}(P)$ as

$$\text{IND}(P) = \{(x, y) \in U \times U \mid \forall a \in P, a(x) = a(y)\} \quad (1)$$

- $\text{IND}(P)$ generates a partition of U, denoted with U/P
- If $(x, y) \in \text{IND}(P)$, then x and y are indistinguishable w.r.t. the attributes in P, i.e, they are *p-indistinguishable*

Pawlak rough set model

- Represent set X such that $X \subseteq U$ using P (where $P \subseteq A$)
- X can be approximated by using *lower* and *upper approximation*:

$$\underline{P}X = \{x \mid [x]_P \subseteq X\} \quad (2)$$
$$\overline{P}X = \{x \mid [x]_P \cap X \neq \emptyset\} \quad (3)$$

  where $[x]_P$ denotes the equivalence classes of the p-indistinguishability relation
- Lower approximation is the set of objects that are positively classified as being members of set X, i.e., union of all equivalence classes in $[x]_P$
- Upper approximation is the set of objects that are possibly in X
- Its complement, $U - \overline{P}X$, is the negative region with sets of objects that are definitely not in X (i.e., $\neg X$)

Pawlak rough set model

- With every rough set, we associate two *crisp* sets (the *lower* and *upper approximation*), denoted as a tuple $X = \langle \underline{X}, \overline{X} \rangle$
- Boundary region $B_P X = \overline{P}X - \underline{P}X$, where its objects neither can be classified as to be member of X nor that they are not in X
- If $B_P X = \emptyset$ then X is, in fact, a crisp set with respect to P and when $B_P X \neq \emptyset$ then X is rough w.r.t. P.
- Accuracy of approximation, reduct (sufficient conditions), core (necessary conditions), and

$$\underline{P}X \subseteq X \subseteq \overline{P}X \quad (4)$$

Example: second-hand vehicles

	Age	Wheels	Engine	Helmet
o_1	< 5	2	no	no
o_2	> 5	2	no	no
o_3	> 5	2	yes	yes
o_4	> 5	3	yes	yes
o_5	> 5	3	yes	yes
o_6	> 5	3	no	yes
o_7	> 5	3	no	no
o_8	< 5	2	no	no
o_9	< 5	4	yes	no

Induced equivalence classes:

$[\text{one}] = \{o_1, o_8\}$ $[\text{four}] = \{o_4, o_5\}$
$[\text{two}] = \{o_2\}$ $[\text{five}] = \{o_6, o_7\}$
$[\text{three}] = \{o_3\}$ $[\text{six}] = \{o_9\}$

Rough sets for our vehicles

- Assume our target set X has members $\{o_3, o_4, o_5, o_6\}$
- Then [*four*] and [*three*] are *definitely* in out target set, i.e., is the *lower approximation* $\underline{X} = \{o_3, o_4, o_5\}$
- But what about o_6?
- Given [*five*] $= \{o_6, o_7\}$, we cannot distinguish between o_6 and o_7, so [*five*] as such cannot be part of our target set, i.e., with the given (incomplete?) information, there is no way to represent X such that it includes o_6 but excludes o_7
- *Upper approximation* of X is $\overline{X} = \{o_3, o_4, o_5, o_6, o_7\}$
- *Boundary region*: $\{o_6, o_7\}$
- 'heuristic': once there are equivalence classes with more than one object, there likely will be at least one rough set

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Reduct and core

- Reduct can be considered to be the set of *sufficient* conditions (attributes) to maintain the equivalence class structure induced by P
- Core can be considered to be the set of *necessary* conditions to maintain the equivalence class structure induced by P
- $\textsc{Core} \subseteq \textsc{Red} \subseteq P$ such that $[x]_{\textsc{Red}} = [x]_P$ and $\textsc{Red}$ is minimal for any $a \in \textsc{Red}$ (i.e., $[x]_{\textsc{Red}-\{a\}} \neq [x]_P$)
  - That is, those attributes that are in P but not in $\textsc{Red}$ are superfluous with respect to the partitioning with P
- For any reduct of P, $\textsc{Red}_1, \ldots, \textsc{Red}_n$, the core is its intersection, i.e., $\textsc{Core} = \textsc{Red}_1 \cap \ldots \cap \textsc{Red}_n$
  - No attribute in $\textsc{Core}$ can be removed without destroying the equivalence structure
  - It is possible that $\textsc{Core}$ is an empty set

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From ‘information system’ to DLs

- More constructors and possible constraints in a DL-ontology, notably a set of roles, $\mathcal{R}$, over objects quantification, role properties
- More flexibility on representing ‘attributes’ of a concept $C \in \mathcal{C}$: either with one or more roles $R \in \mathcal{R}$ or value attributions $D \in \mathcal{D}$, or both
- Need for a complete and appropriate model-theoretic semantics for $\underline{C}$ and $\overline{C}$, and the rough concept, denoted with “$\wr C$”
- Given that attributes are used to compute $\underline{C}$ and $\overline{C}$, then those attributes must be represented in the DL KB, and with $\wr C$ a tuple of the former two, then also it must have those attributes

On the semantics of $\wr C$

- Lower and upper approximation:

$$\underline{C} = \{x \mid \forall y : (x,y) \in Ind \rightarrow y \in C\} \qquad (5)$$
$$\overline{C} = \{x \mid \exists y : (x,y) \in Ind \land y \in C\} \qquad (6)$$

- $\wr C = \langle \underline{C}, \overline{C} \rangle$
- Interpretation maps every $\wr C = \langle \underline{C}, \overline{C} \rangle$ to a pair over $\Delta^{\mathcal{I}}$, i.e., extending $\cdot^{\mathcal{I}}$ as follows:

$$\wr C^{\mathcal{I}} = (\langle \underline{C}, \overline{C} \rangle)^{\mathcal{I}} = \langle (\underline{C})^{\mathcal{I}}, (\overline{C})^{\mathcal{I}} \rangle \qquad (7)$$

- Subsumption relation between the sets as in (4) and their corresponding concepts, but does not *define* it
- Make explicit the knowledge about the three sets and how they relate

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On the semantics of $\wr C$

- Introduce two binary relationships, *lapr* and *uapr*, to relate *any* rough concept and its associated approximations

$$\forall \phi, \psi . lapr(\phi, \psi) \rightarrow \wr C(\phi) \wedge \underline{C}(\psi) \quad (8)$$
$$\forall \phi, \psi . uapr(\phi, \psi) \rightarrow \wr C(\phi) \wedge \overline{C}(\psi) \quad (9)$$

- Make explicit that $\wr C$ is identified by the combination of its $\underline{C}$ and $\overline{C}$:

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&\forall \phi . \wr C(\phi) \rightarrow \exists \psi . lapr(\phi, \psi), \\
&\forall \phi . \wr C(\phi) \rightarrow \exists \psi . uapr(\phi, \psi), \\
&\forall \phi, \psi, \varphi . lapr(\phi, \psi) \wedge lapr(\phi, \varphi) \rightarrow \psi = \varphi, \quad (10) \\
&\forall \phi, \psi, \varphi . uapr(\phi, \psi) \wedge uapr(\phi, \varphi) \rightarrow \psi = \varphi, \\
&\forall \phi_1, \phi_2, \psi_1, \psi_2 . lapr(\phi_1, \psi_1) \wedge uapr(\phi_1, \psi_2) \wedge \\
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Further requirements

- In the DL KB, the set of 'attributes' amounts to $\mathcal{R} \cup \mathcal{D}$
- Impose that those attributes P taken from $\mathcal{R} \cup \mathcal{D}$ must be represented in the ontology with $\wr C$ as its domain
- The indistinguishability relation is reflexive, symmetric, and transitive

Related works

- DL or OWL ontologies:
  - More precise notion of $\wr C$ cf. the tuple notation [JWTX09]
  - Use both $\mathcal{R}$ and $\mathcal{D}$ for the 'attributes' (properties) of the concepts cf. $\mathcal{R}$ only in [IGNI07, SKP07]
  - Include the properties of the indistinguishability relation cf. their omission in [Lia96] or using the properties of the similarity relation [BS09]
  - Adhere to proper $\underline{C}$, $\overline{C}$, and $\wr C$ in that they all have the same collection of properties from $\mathcal{R} \cup \mathcal{D}$ cf. the 'approximations' with different sets of attributes in [SKP07]
- Other formalisations:
  - Propositional: [D97, KB08, Nak96]
  - Data/logical level: with DATALOG [DLSS06] or extended logic programs [VDM03]

Core issues for a rough DL KB

- Identification of the rough concept
  - Second order logic
  - **id** constraint in the language ($\mathcal{DLR}_{ifd}$, *DL-Lite*$_{\mathcal{A},id}$)
  - Let each rough concept be subsumed by some "`RoughC`" to communicate with the modeller it is intended as a rough concept
- Properties of the indistinguishability relation ($\mathcal{SROIQ}$, $\mathcal{DLR}_{\mu}$)
- Reasoning: possibly and definitely satisfiable, rough subsumption, and instance classification
- Scalable non-empty ABox to figure out if some concept is actually a rough concept or not (*DL-Lite* family)

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Three experiments

- Promiscuous bacteria with OBDA and a operational database (HGT-DB [GVGMR03] using set up described in [CKN+10] and OBDA plugin for Protégé for querying)—**to find vague instances**
- Promiscuous bacteria with the expressive ontology language OWL 2 DL and Protégé—**to model the rough concepts**
- Revisiting Septic patients example [JWTX09, SKP07] to give the Protégé with OWL 2 DL a fairer chance and use RacerPro 2 Preview too—**To model rough concepts, with complex definitions, and find vague instances in the few objects in the ABox**
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Procedure (1/2)

1. Develop a basic ontology in OWL 2 QL or *DL-Lite*$_{\mathcal{A}}$ stored as an OWL file;
2. Obtain the relational database in Oracle, DB2, MySQL, or PostgreSQL;
3. Set up the OBDA system with the QuOnto reasoner, Protégé, and OBDA plugin for Protégé;
4. Declare the mappings between the classes and properties in the ontology and SQL queries over the database in the OBDA plugin for Protégé;
5. Find all rough concepts with respect to the data through posing ontology-mediated queries (in SPARQL or EQL-Lite), evaluating the result set, and adding them to the ontology;

Procedure (2/2)

6. Migrate this ontology to an expressive OWL species, such as OWL 2 DL, by:
    i. Declaring the semantics from the WHERE clause in the SQL query of the mapping layer as object and data properties in the ontology;
    ii. Adding upper and lower approximations of each rough concept;
    iii. Adding the indistinguishability object property with its properties (reflexive, symmetric, transitive);
    iv. Adding the axioms relating the approximations to the rough concepts and vice versa;
7. When the rough reasoning services are implemented, run the reasoner with the enhanced ontology to check satisfiability and consistency

On step 6 of the procedure

- Recollecting the relevant part of OWL 2's direct semantics [MPSG09]: take a vocabulary V with, among others,
  i. V_C denotes the set of classes
  ii. Class interpretation function $\cdot^C$ assigns to each class $C \in V_C$ a subset $(C)^C \subseteq \Delta^I$
  iii. V_{OP} the set of object properties
  iv. $\cdot^{OP}$ is the object property interpretation function that assigns to each object property $OP \in V_{OP}$ a subset $(OP)^{OP} \subseteq \Delta^I \times \Delta^I$
- Add rough concept, upper, and lower approximation such that $\wr \mathtt{C}, \overline{\mathtt{C}}, \underline{\mathtt{C}} \in V_C$

On step 6 of the procedure (Cont'd)

- add the indistinguishability relation Ind over $\Delta^I \times \Delta^I$ as an object property such that $\texttt{Ind} \in V_{OP}$ and the ontology contains the assertions:
  `ReflexiveObjectProperty(a:Ind)`,
  `SymmetricObjectProperty(a:Ind)`, and
  `TransitiveObjectProperty(a:Ind)`
- assign the semantics to the classes:

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\begin{aligned}
(\overline{\mathtt{C}})^I &= \{x \in \Delta^I \mid \exists y \in \Delta^I, (x,y) \in \mathtt{Ind} \wedge y \in \mathtt{C}^I\} \\
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(\wr \mathtt{C})^I &= (\langle \underline{\mathtt{C}}, \overline{\mathtt{C}} \rangle)^I = \langle (\underline{\mathtt{C}})^I, (\overline{\mathtt{C}})^I \rangle
\end{aligned} \tag{11}
$$

which amounts to the assertions for any $\overline{\mathtt{C}}$ and $\underline{\mathtt{C}}$ in OWL 2 DL functional syntax:
`EquivalentClasses(C̄ ObjectSomeValuesFrom(a:Ind a:C))` and
`EquivalentClasses(C̲ ObjectAllValuesFrom(a:Ind a:C))`

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- (11) is approximated in an arbitrary ontology by adding two auxiliary roles, `uapr`, `lapr` $\in V_{OP}$ that each have ≀C as domain, and cardinality exactly 1:
  `ObjectPropertyDomain(a:upar a:≀C)`,
  `ObjectPropertyDomain(a:lapr a:≀C)`,
  `ObjectExactCardinality(1 a:uapr a:`$\overline{\texttt{C}}$`)`, and
  `ObjectExactCardinality(1 a:lapr a:`$\underline{\texttt{C}}$`)`.
- All this is added to the expressive ontology for each rough concept

On step 6 of the procedure (Cont'd)

- (11) is approximated in an arbitrary ontology by adding two auxiliary roles, `uapr`, `lapr` $\in V_{OP}$ that each have $\wr$C as domain, and cardinality exactly 1:
  ObjectPropertyDomain(a:upar a:$\wr$C),
  ObjectPropertyDomain(a:lapr a:$\wr$C),
  ObjectExactCardinality(1 a:uapr a:$\overline{\text{C}}$), and
  ObjectExactCardinality(1 a:lapr a:$\underline{\text{C}}$).
- All this is added to the expressive ontology for each rough concept

Materials

- OBDA: Oracle 10g RDMBS, QuOnto, Protégé 3.3.1, OBDA Plugin for Protégé
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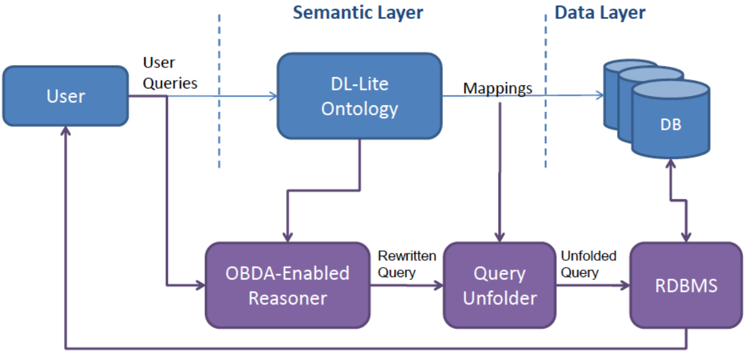
Section of the ORM version of the HGT model



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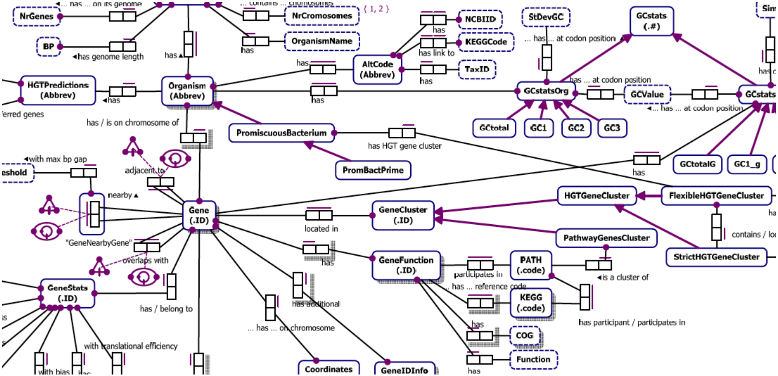

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OBDA and QuOnto

- Promiscuous bacterium is a Organism and, **putatively**, it must have more than 5 flexible hgt-gene clusters and the percentage of genes on the chromosome that are predicted to be horizontally acquired as > 10
- Head of the mapping:
  PromiscuousBacterium(getPromBact($abbrev,$ccount, $percentage))
- Body:
  ```
  SELECT organisme.abbrev, ccount, organisme.percentage
  FROM ( SELECT idorganisme, COUNT(distinct cstart)
  as ccount FROM COMCLUSTG2 GROUP BY idorganisme
  ) flexcount, organisme
  WHERE organisme.abbrev = flexcount.idorganisme AND
  organisme.percentage > 10 AND flexcount.ccount > 5
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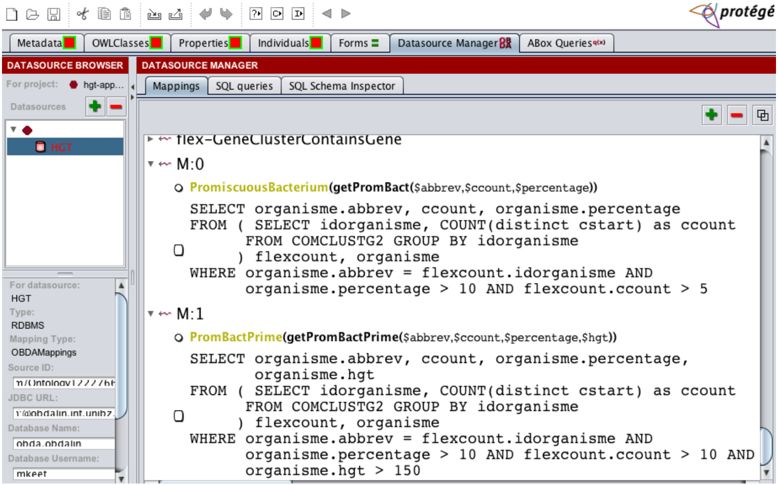
Mappings


protégé
Metadata
OWLClasses
Properties
Individuals
Forms
Datasource Manager
ABox Queries
DATASOURCE BROWSER
For project:
hgt-app...
Datasources
HGT
For datasource:
HGT
Type:
RDBMS
Mapping Type:
OBDAMappings
Source ID:
JDBC URL:
Database Name:
obda.obdalin
Database Username:
mkeet
DATASOURCE MANAGER
Mappings
SQL queries
SQL Schema Inspector
flex-GeneClusterContainsGene
M:0
PromiscuousBacterium(getPromBact($abbrev,$ccount,$percentage))
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organisme.percentage > 10 AND flexcount.ccount > 5
M:1
PromBactPrime(getPromBactPrime($abbrev,$ccount,$percentage,$hgt))
SELECT organisme.abbrev, ccount, organisme.percentage,
organisme.hgt
FROM (SELECT idorganisme, COUNT(distinct cstart) as ccount
FROM COMCLUSTG2 GROUP BY idorganisme
) flexcount, organisme
WHERE organisme.abbrev = flexcount.idorganisme AND
organisme.percentage > 10 AND flexcount.ccount > 10 AND
organisme.hgt > 150

Promiscuous bacteria with OBDA and QuOnto

- Query the HGT-DB through the ontology with a SPARQL query:
  - 98 objects are retrieved where *Dehalococcoides CBDB1* and *Thermotoga maritima* are truly indistinguishable bacteria, i.e. they have the same values for all the selected and constrained attributes
  - A few others are very close to being so, e.g., *Pelodictyon luteolum DSM273* and *Synechocystis PCC6803* who have both 6 clusters and 10.1% and 10.2%, respectively
- Refine to Prombact′ to check if we can obtain a crisp concept

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Promiscuous bacteria with OWL 2 DL

Add definitions

$$PromBact \equiv Organism \sqcap \exists\, Percentage.real_{>10} \sqcap \geq 6\ hasHGTCl.FlexibleHGTGeneCl \quad (12)$$

$$PromBact' \equiv PromBact \sqcap \exists\, Percentage.real_{>10} \sqcap \geq 11\ hasHGTCl.FlexibleHGTGeneCl \sqcap \exists\, NrPredHGTgenes.integer_{>150} \quad (13)$$

and rough concept notions (14-17) with their relational properties **only for the rough concept**:

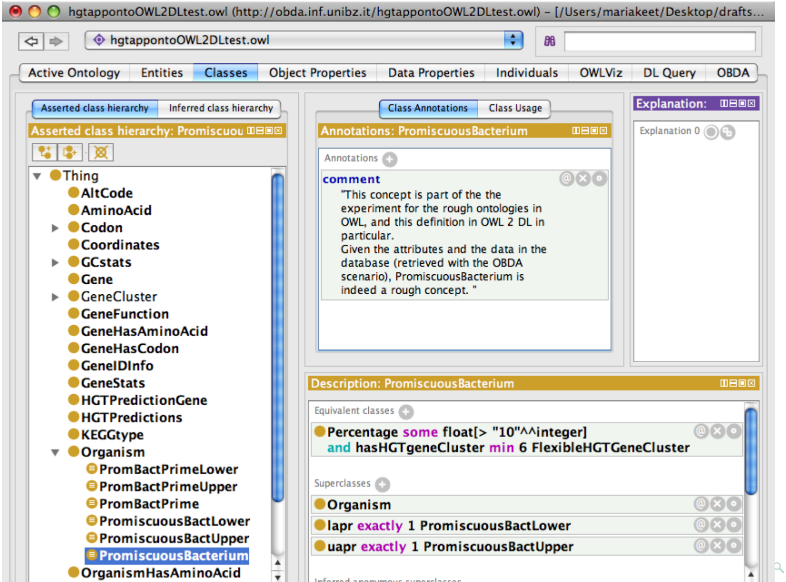
$$PromBact \sqsubseteq\ = 1\ lapr.PromBactLapr \quad (14)$$

$$PromBact \sqsubseteq\ = 1\ uapr.PromBactUapr \quad (15)$$

$$PromBactLapr \equiv \forall\, ind.PromBact \quad (16)$$

$$PromBactUapr \equiv \exists\, ind.PromBact \quad (17)$$

In Protégé 4.0



Bone and strict septic

Patients may be septic or are certainly septic, according to the so-called *Bone criteria* and Bone criteria together with three out of another five criteria, respectively; e.g., the Bone criteria (from [SKP07]):

- *Has infection;*
- *At least two out of four criteria of the Systemic Inflammatory Response Syndrome:*
  - *temperature* $> 38^\circ C$ *OR temperature* $< 36^\circ C$*;*
  - *respiratory rate* > 20 *breaths/minute OR* $PaCO_2 < 32$ *mmHg;*
  - *heart rate* > 90 *beats/minute;*
  - *leukocyte count* $< 4000\ mm^3$ *OR leukocyte count* $> 12000\ mm^3$*;*
- *Organ dysfunction, hypoperfusion, or hypotension.*

Bone septic in OWL

can be encoded in OWL in Protégé as being an `EquivalentClass` to `BoneSeptic`, as follows:

```
(hasDiagnosis some Infection and
hasSymptom some (Hypoperfusion or Hypotension or OrganDysfunction)
and (((temperature some int[> 38] or temperature some int[<36])
and (respiratoryRate some int[>20] or paco2count some int[<32]))
or ((temperature some int[>38] or temperature some int[<36]) and
heartRate some int[>90])
or ((temperature some int[>38] or temperature some int[<36]) and
(leukocyteCount some int[<4000] or leukocyteCount some int[>12000]))
or ((respiratoryRate some int[>20] or paco2count some int[<32]) and
heartRate some int[>90])
or ((respiratoryRate some int[>20] or paco2count some int[<32]) and
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or (heartRate some int[>90] and (leukocyteCount some int[<4000] or
leukocyteCount some int[>12000]))))
```

Results

- Definitions and encodings in Protégé 4.0 and RacerPro 2.0 preview and data of 17 'patients' s.t. the boundary region of each concept is not empty are available through `http://www.meteck.org/files/roughontosuppl/roughontotests.html`
- Protégé 4.0 with Pellet 2.0 did not work at all
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Discussion

- Ontologies, OBDA, and ontology development tools provide a means to deal with successive de-vagueing during experimentation
- Makes the iterations with the selected properties explicit
- The two-step process with OBDA and OWL 2 DL is an advance w.r.t. traceability
- Meaningful and usable language extensions for a proper rough DL are limited, reasoning services can be augmented
- Other options:
  - At least: partition the data source;
  - Sophisticated modularization of both the ontology and the data(base) (e.g., [LTW09, BBLW10])
  - Turn the 'methodology' into a structured scientific workflow to be able to seamlessly go back and forth between OBDA and OWL 2 DL

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Conclusions and future directions

- Given rough sets' semantics, there is no, nor will there be, a DL that represents all essential aspects precisely, though $\mathcal{SROIQ}(\mathcal{D})$ is fairly close
- Interaction with large amounts of data that makes any extension with roughness interesting and useful, e.g., the *DL-Lite* family with its OBDA infrastructure
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Thank you for your attention