

Shadowboxing: Mirroring the TBox in the ABox

Christopher J. Mungall^{1*}

¹Genomics Division, Lawrence Berkeley National Laboratory, MS84R017, 1 Cyclotron Road, Berkeley, CA 94720 USA

ABSTRACT

OWL2 has a strict separation between classes (TBox) and the domain of discourse (ABox). This separation generally works well for the tasks that OWL is designed for, but there are scenarios where it is desirable to model simultaneously as classes and individuals. This can also have advantages when mapping an OWL TBox to graph representations such as RDF, where the standard mapping produces a striping pattern that does not align well with conventional graph representations.

In this document we describe a method for modeling an OWL TBox inside an ABox that is *valid* with respect to the original ontology, allows additional entailments, and provides a more useful substrate for graph traversal than the standard OWL RDF mapping.

1 INTRODUCTION

1.1 ABoxes and TBoxes

With traditional Description Logics, objects can belong to either the TBox (“terminology” box, i.e. set of *classes*), the ABox (“assertion” box, i.e. set of *individuals*) or the RBox (the set of *properties*)¹. The ABox is also known as the *domain of discourse*. These two sets do not share members; OWL2 introduces the notion of *punning*, whereby the same name (i.e. IRI) can refer to either a class or individual, but this is just a syntactic convenience for sharing annotations. Logically, a punned name is in fact two names, and the ABox-TBox distinction is thus maintained.

The modeler must decide how to partition their objects of interest into the TBox and ABox. In general, units of classification (i.e. classes) should be modeled in the TBox as OWL classes, as this can maximally leverage OWL tooling. For example, an ontology may contain a class “hippocampus”, representing the set of all hippocampi; it would be unusual for an OWL ontology to have an *individual* named “hippocampus”.

The choice is not always straightforward. In the biological domain, valid arguments exist for whether objects such as *gene* or *species* should be modeled in the ABox or TBox, and the modeler may be guided by a variety of considerations, including philosophical principles or practical modeling consequences based on the constraints imposed by the choice.

Modeling in the ABox provides certain advantages - if the objects are in the domain of discourse they are more readily queryable. Certain limitations can be bypassed such as the tree model property of OWL TBoxes - for example, it is impossible to model a cyclic molecule in an OWL TBox (see Dumontier 2007[?]), so there

may be practical advantages in modeling chemical structures such as “benzene” in the ABox.

1.2 OWL, RDF and Graphs

Ontologies are commonly conceived of as graphs; for example, the seminal Gene Ontology paper[1] uses the datamodel of a Directed Acyclic Graph, and most bioinformatic tools and relational databases use a graph model to represent the ontology[?]. Here, each class is mapped to a vertex V in the graph, with each axiom connecting two classes being mapped to an edge E , with the ontology being mapped to the graph G , where $G = \langle V, E \rangle$.

RDF (Resource Description Framework) is a subset of first-order logic consisting of “subject-predicate-object triples” i.e. predicate sentences with two arguments. This has a natural mapping to graphs, with each triple forming an edge E .

An OWL ontology can be represented as an RDF graph, i.e. a set of triples. There is a standard serialization into triples provided by the W3 recommendation *mapping to rdf*².

Following this serialization, a single existential axiom of the form³:

```
X SubClassOf R some Y
```

Is mapped to 4 triples⁴

```
X rdfs:subClassOf _:1 .
_:1 a owl:Restriction .
_:1 owl:onProperty R .
_:1 owl:someValuesFrom Y /
```

This can become verbose where ontologies contain multiple such existential axioms (as is standard for most bio-ontologies - e.g. partonomies in anatomical ontologies). This can be a hindrance when working with ontologies using RDF tools that do not support an OWL syntactic sugar layer, or in using technologies designed for reasoning over triples.

It is also problematic when the RDF representation of the OWL is directly mapped to a graph when using graph-based software (e.g. visualization tools such as cytoscape or graph databases such as Neo-4j). This is because the “striping” above essentially produces a bipartite graph, rather than a “clean” graph as outlined above.

Many knowledge bases (e.g. freebase; neurolex) use a simple form of knowledge representation where concepts are linked via triples, eschewing more formally specified OWL axioms and attendant reasoning benefits.

*to whom correspondence should be addressed

¹ other object types not relevant for this paper

² <http://www.w3.org/TR/owl2-mapping-to-rdf/>

³ We use Manchester Syntax to write OWL axioms

⁴ We use n-triples format to write RDF

We may be tempted to map an OWL ontology to triples in a more direct fashion:

```
X SubClassOf R some Y <==> <X R Y> .
```

The problem with this naive translation is that it leads to *incoherent* ontologies - i.e. ontologies that contain unsatisfiable classes. E.g. consider the following biologically accurate and coherent 4-axiom ontology:

```
Class: nucleus
  SubClassOf: hasPart some chromosome
Class: mitochondrion
  SubClassOf: hasPart some chromosome
ObjectProperty: hasPart
  InverseOf: partOf
Axiom:
  (partOf some nucleus)
    DisjointWith
  (partOf some mitochondrion)
```

The first two axioms⁵ are translated as

```
<nucleus hasPart chromosome> .
<mitochondrion hasPart chromosome> .
```

Because of the inverse properties axiom we entail

```
<chromosome partOf nucleus> .
<chromosome partOf mitochondrion> .
```

If we translate these back to OWL using the naive translation, we end up with an incoherent ontology (because *nucleus* and *chromosome* are entailed to be equivalent to Nothing):

```
Class: chromosome
  SubClassOf: partOf some nucleus
  SubClassOf: partOf some mitochondrion
ObjectProperty: hasPart
  InverseOf: partOf
Axiom:
  (partOf some nucleus)
    DisjointWith
  (partOf some mitochondrion)
```

Even when translating in one direction, we can end up with undesired inferences (e.g. consider domain and range constraints).

Despite this problem, the naive translation is sometimes used where there is a desire to have a simpler RDF representation.

1.3 Requirements for a graph mapping of OWL2

Our requirements for a mapping from OWL2 to a graph are:

1. aligns with a basic graph representation (does not introduce blank nodes and striping)
2. coherency-preserving
3. preserves entailments where possible
4. supplements standard W3C translation rather than replaces it

⁵ we leave as open for now the question of how to map axioms such as Disjointness axioms

The standard W3C mapping to RDF preserves coherency and many entailments - but violates the first requirement by introducing blank nodes for existential restrictions.

The naive translation succeeds with the first requirement, but fails to preserve coherency (and consequently fails to preserve entailments?).

2 TBOX SHADOWING

We introduce a method called TBox shadowing. This is very similar to the naive translation, but introduces a mapping at the level of object properties to preserve coherency.

2.1 Preliminaries

2.1.1 Graphs

2.1.2 RDF

2.1.3 OWL-DL

2.1.4 OWL-Full

2.2 Translation of Class Axioms

Each class C in O is mapped a named individual C in O' . The same name (IRI) is used - this means that if O and O' are combined we have *emphunning*.

A subset of class axioms in O are translated to ObjectPropertyAxioms in O'

```
A SubClassOf B ==> OPE(A SubClassOf' B)
A SubClassOf R some B ==> OPE(A R' B)
```

Strictly speaking the A and the B classes on the LHS are different objects from the A and B individuals on the RHS, but we use OWL2 punning in our notation here.

Here R' denotes a type-level counterpart or shadow of R . Note that punning is *not* used here R' is a truly distinct name (IRI) from R . Both R and R' are ObjectProperties.

SubClassOf' is an OWL2-DL ObjectProperty that is a type-level counterpart of the RDFS/OWL-Full `rdfs:subClassOf` property

We introduce two property chain axioms for every shadowed property R' :

```
R' o SubClassOf' ==> R'
SubClassOf' o R' ==> R'
```

Together with:

```
Transitive(SubClassOf')
Reflexive(SubClassOf')
AntiSymmetric(SubClassOf')
```

To illustrate, consider an ontology O' is:

```
A SubClassOf B
B SubClassOf partOf some C
C SubClassOf D
```

Then O' entails

```
<A partOf' D>
```

2.2.1 Conherency Proof TODO: Proof that this is coherency-preserving. Intuitively this is the case as subclass inferences propagate over existentials.

2.3 Translation of Object Property Axioms

A subset of axioms for R are also shadowed:

```
Transitive(R) ==> Transitive(R')
R <- R1 o ... o Rn ==> R' <- R1' o ... o Rn'
```

2.3.1 Conherency Proof TODO: Proof that this is coherency-preserving

2.3.2 Propagation of symmetry axioms introduces incoherency TODO: Example. E.g. nucleus adjacentTo cytoplasm.

2.3.3 Propagation of inverse axioms introduces incoherency See example in introduction

2.4 Translation of equivalence axioms

Equivalence axioms currently have an incomplete translation. Currently only "genus-differentia" style are translated:

```
X = G and R1 some Y1 and ..
==>
X sameAs GenId
GenId SubClassOf' G
GenId R1' Y1,
....
```

Where GenId is an auto-generated IRI (e.g. using a UUID) to avoid falling outside OWL2

TODO: this relies on CWA, need to explicitly close the world

2.5 Translation of annotation axioms

Because the same names (IRIs) are used for classes, each class C in O' should have the same annotations, if O' extends O .

However, care must be taken in copying annotations from an object property R to its shadow R' .

Annotations are logically silent, so propagation will not affect entailment. However, annotations should not be propagated blindly as this could cause confusion. We recommend some kind of syntactic pattern for translation of object property annotations involving certain annotation properties such as `rdfs:label`.

3 IMPLEMENTATION

A preliminary implementation is available in OWLTools⁷.

The class name is `owltools.mooncat.OWLInABoxTranslator`⁸

To run:

```
owltools my.owl --tbox-to-abox -o my-abox.owl
```

The translation by default generates label annotations for shadowed object properties, suffixing them with "type level".

The method `trTypeLevel` will generate a name R' shadowing an object property R . Currently it does this by suffixing the IRI with the string "TLR", but in future this may be configurable.

The `SubClassOf` object property is the same translation applied to the IRI for `rdfs:subClassOf` (this may be changed in the future).

4 OWL2 PROFILE OF SHADOWED TBOX

The shadowed TBox falls in the EL++ subset, which allows use of fast reasoners such as Elk.

In addition, the kinds of simple entailment supported by many triplestores becomes more useful with a shadowed TBox in comparison to the W3C translation.

Note that shadowing loses axioms. For many applications this may not matter. For example, an ontology O can be validated and pre-classified using OWL reasoners, with direct inferred axioms added to make O_2 , and then applications consume O'_2 .

5 APPLICATIONS

5.1 SPARQL queries

The standard W3C mapping of OWL to RDF results in additional blank nodes and striping, making basic SPARQL queries difficult. In addition, the simple entailment regimes provided with some SPARQL engines may be incapable of basic inferences, such as those combining transitivity of object properties and existential axioms. These are at the core of many biological ontologies, which often have a partonomy as the backbone (e.g. neuro-anatomy), or sometimes an ontogenic lineage (e.g. cell ontologies).

For these reasons, many triplestores eschew an OWL2 TBox representation, and use triples to connect the representational units. This is typically done in an ad-hoc way without thought to the OWL2 semantics, sometimes resulting in accidentally falling into OWL-Full, sometimes limiting the use of the knowledge base for complex queries etc. Examples include dbpedia, freebase, the neurolex triplestore. The Non-DL OWL translation of the FMA can be considered to fall into this category.

TODO - compare queries.

TODO - example query from Neurolex paper

5.2 Mapping to graph databases

TBox shadowing provides one way to map an OWL ontology to graph databases such as Neo4j, and to graph-based visualization tools such as Cytoscape.

Whilst it would be possible to simply use the naive translation (Neo4j models do not have a formal set-theoretic or first order logic interpretation, so there is no danger of introducing incoherency), using the TBox shadowing mapping has the advantage of having a simultaneous direct RDF translation of the Neo4j that is coherent. The cost is the introduction of an object property mapping.

Non-RDF graph models often allow multiple labels, so another alternative is to annotate the edge with logical properties. For example, an existential restriction axiom may be mapped to a single edge annotated with both the object property and the expression type (`ObjectSomeValuesFrom`).

⁷ <http://owltools.googlecode.com>

⁸ <http://owltools.googlecode.com/svn/trunk/docs/api/owltools/mooncat/OWLInABoxTranslator.html>

5.3 Formalization of Type-Level Relations

The OBO Relations Ontology paper from 2005[3] formalized a set of binary type level relations in terms of instance-level binary or ternary (time-indexed) relations. In this formalization, classification units such as “cell” and “cell nucleus” are conceived of as “types” or “universals”, and are considered to be part of the domain of discourse.

For example, the logic sentence “CellNucleus *part of* Cell” (using the 2-argument type-level part-of relation) has an interpretation:

$$\forall x \forall t : \text{instance_of}(x, \text{cell nucleus}, t) \rightarrow \\ \exists y \text{instance_of}(y, \text{cell}, t), \text{part_of}(x, y, t)$$

There is no agreed-upon alignment of the RO 2005 paper with OWL. Whilst the type-level relationships (such as that between nucleus and cell) might naturally be represented using a single triple, this was generally eschewed by ontologies using OWL, and instead existential restrictions were used[2], in order to maximize use of OWL and OWL reasoners. However, this approach has problems as it introduces binary instance-level relations whose temporal interpretation is not clear.

The TBox shadowing strategy outlined in this document could be used to provide a partial alignment of RO-2005 to OWL.

Here, the RO-2005 notion of “type level relation” corresponds directly to shadowed object properties, and the punned class names correspond to universals/types (which are in the domain of discourse).

Under this interpretation, the shadowed TBox axioms in the ontology O' would be conceived of as the primary or canonical OWL representation of the ontology. The corresponding TBox representation would be conceived of as a derived artifact that can be used in conjunction with OWL tools and OWL reasoners.

This is just a preliminary sketch of the approach - it does not address time-indexed instance level relations, and it leaves open the possibility of different kinds of temporal quantification for the type level relations (e.g. there may be a TLR for at-some-times as well as at-all-times).

5.4 Phylogenetic trees

5.5 Anatomical structures and homology

A standard OWL2 anatomical ontology uses classes to represent generalizations of particular anatomical structures in the world. For example, the class “finger” is instantiated by all actual fingers, such as my left middle finger.

This is obviously useful for OWL reasoning, but placing the generalized structures outside the domain of discourse has some consequences when the generalized structures are themselves the subject of study as opposed to groupings for data.

For example, evolutionary developmental biology is concerned with how structures such as the limb or the digits have changed (or are preserved) over deep time. In a conventional TBox representation, all class axioms hold over the individual structures themselves - my left forelimb, the pectoral fin of this particular fish instance - not about the patterns observed at the level of individual species. Homology is often conceived of in terms of these patterns (Van Valen).

One practical consequence is in recording homology statements. With a TBox representation, the axiom

```
forelimb SubClassOf
```

```
homologousTo some 'pectoral fin'
```

does *not* entail:

```
'pectoral fin' SubClassOf
  homologousTo some forelimb
```

This is somewhat unsatisfactory, as we are forced to make reciprocal assertions (there are no situations where the reciprocal axiom would not be true). This is not a major issue, something easily addressed with a patina of additional tooling. But it does hint that we are working at the wrong level of abstraction and we need the anatomical structures to be in the domain of discourse. Then we could simply write:

```
OPE(forelimb homologousTo 'pectoral fin')
Symmetric(homologousTo')
```

And get the correct entailments.

The TBox shadowing provides a mechanism for doing this. Anatomy ontologies can continue to be authored as conventional TBox ontologies. Entailments from O' can be reverse-shadowed back into O (giving a more formal mechanism for ensuring TBox homology axioms are reciprocated). Or in fact O' could be regarded as the canonical representation. This has some philosophical appeal, if one conceives of evolution as being about changes in patterns.

There may be additional expressivity gains beyond symmetry of assertions. MORE TO BE WRITTEN HERE

5.6 Genes and proteins

There are various tradeoffs when deciding whether to model specific genes (such as “human alpha-synuclein gene”) in the TBox or ABox. Some are fairly prosaic yet important - e.g. if the TBox is conceived of by some tools as the “terminology box” then a TBox representation allows use of some terminology tools. Other reasons pertain to the kinds of entailments desired and the kinds of questions asked. Or an approach based in ontological realism may be preferred, with distinctions drawn between physical molecule regions, information content entities, and mind-independent generically dependent continuants.

To see some of the practical considerations, consider a TBox model (for example, the PRO ontology, which is class based, with the individuals being actual protein molecule instances - one can easily conceive of a gene parallel to this).

How do we answer the question “how many genes does a human have”? This question is strictly speaking underspecified - one could answer with the number of distinct physical DNA portions with coding potential in a given human, which would be in the trillions. But this would be perverse. Typically we are interested in the interpretation that yields an answer of the order 20-30k (ignoring for now interesting but not relevant questions of biochemically active but unselected DNA, etc).

It is difficult to get a TBox model to yield this answer. The reason being we are implicitly interested in a particular level of specificity - SHH, SNCA, PINK1, ... these are all “distinct” genes at the right level of specificity. “developmental gene” or “synuclein family gene” are not - yet these are valid classes in the TBox model.

THIS IS GETTING TOO WAFFLY...

ADD EXAMPLE INVOLVING PHYLOGENETIC TREES

6 DISCUSSION

Even in an OWL environment, answering questions such as "what are the descendants of 'finger'" and receiving a `part_of` edge to 'limb' are not directly supported in OWL reasoners - it is necessary to materialize R-some-Y classes.

More generally, because classes are part of the TBox and not in the domain of discourse, certain kinds of queries are harder. These include queries for homologous structures, where these structures are traditionally represented as classes.

7 CONCLUSIONS

REFERENCES

- [1]M. Ashburner et al. Gene ontology: tool for the unification of biology. The Gene Ontology Consortium. *Nat Genet*, 25(1):25–29, May 2000.
- [2]C. Golbreich and I. Horrocks. The obo to owl mapping, go to owl 1.1. In *Proceedings of the OWLED 2007 Workshop on OWL: Experiences and Directions: June 6-7 2007; Innsbruck, Austria*, 2007.
- [3]B. Smith, W. Ceusters, J. Kohler, A. Kumar, J. Lomax, C.J. Mungall, F. Neuhaus, A. Rector, and C. Rosse. Relations in Biomedical Ontologies. *Genome Biology*, 6(5), 2005.

APPENDIX