

# Building reference alignments for compound matching of multiple ontologies using OBO cross-products

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**Abstract.** Ontology matching techniques are evolving towards more sophisticated approaches, and there is a growing interest in discovering more complex kinds of mappings. Existing techniques are limited to matching two ontologies, but we argue that producing ‘compound’ alignments, involving more than two ontologies, would be useful to support a next generation of semantic technologies.

To foster the development of new techniques in this area, we have investigated the suitability of exploring OBO cross-products to derive ternary compound alignments that can be used as a benchmark. We were able to establish seven such reference alignments with over 100 mappings each, between ten biomedical ontologies. We conducted preliminary experiments to explore the challenges this type of mapping poses for methods commonly used by existing alignment systems. These revealed that the increase in matching space and the inherently more difficult-to-compute ternary mapping pose interesting difficulties to compound ontology matching.

**Keywords:** Ontology Matching, Compound Ontology Matching, Ternary Mapping

## 1 Introduction

Establishing meaningful links between related ontologies is a critical requirement for their interoperability and for realizing the semantic web vision. Throughout the last decade, ontology matching systems have increased in both sophistication and performance [1, 2].

Most ontology matching systems produce equivalence mappings between classes or properties in two ontologies, but in recent years there has been a growing interest in discovering more complex kinds of mappings, such as those between complex concept and property descriptions [3–7]. These can support a number of tasks, including query rewriting [8], and have been identified as one of the future directions for ontology matching [9]. Both the ‘classical’ and ‘complex’

ontology matching approaches focus on discovering mappings between two ontologies. However, in an open, distributed and heterogeneous setting such as the semantic web, to support more elaborate tasks and further improve interoperability it may be advantageous to create mappings by combining entities from more than two ontologies.

We argue that it would be useful for the developers of ontology alignment systems to develop new techniques and tools for identifying 'compound matches', i.e. matches between class or property expressions involving more than two ontologies. The simplest of these mappings would correspond to an equivalence mapping between a class A of one ontology and an expression relating classes B and C of two other ontologies, constituting a ternary relationship. To the best of our knowledge, there are currently no ontology matching systems capable of generating such mappings. One likely reason for this is the lack of an accepted benchmark for measuring a system's performance on identifying this type of mapping. However, several OBO ontologies provide cross-products from which ternary compound mappings can be derived. The purpose of this work is then to investigate the suitability of exploring OBO cross-products to create ternary compound alignments between ontologies. Since OBO cross-products are manually curated, our ultimate goal is to create a set of alignments that can function as a gold-standard to support the evaluation of novel matching methods for compound alignment. We begin the paper by formally defining a compound mapping and describing our approach of leveraging OBO cross-products to create compound mapping reference alignments for several sets of ontologies. Once we have established the reference alignments, we use them to perform a preliminary exploration of the challenges this type of mapping poses for methods commonly used by existing alignment systems.

## 2 Approach

This section introduces the terminology we employ throughout the paper and presents the basics of our approach. We consider that a ternary compound alignment is a set of correspondences (mappings) between classes from a source ontology  $O_s$  and class expressions obtained by combining two other classes each belonging to a different target ontology  $O_{t1}$  and  $O_{t2}$ .

This means that the classic mapping definition, where a mapping belonging to the alignment between ontologies  $O_s$  and  $O_t$  is defined as a triple  $\langle X, Y, M \rangle$ , where X is an entity belonging to  $O_s$ , Y is an entity belonging to  $O_t$  and M is a mapping relation such as equivalence or subsumption, cannot be applied. Instead, we define a ternary compound mapping as a tuple  $\langle X, Y, Z, R, M \rangle$ , where X, Y and Z are classes from three distinct ontologies, R is a relation established between Y and Z to generate a class expression that is mapped to X via a mapping relation M. Here, we consider the ontology to which X belongs to be the source ontology, and the ontologies that define Y and Z to be the target ontologies.

Some of the logical definitions contained in OBO cross-products correspond to

this type of mapping, when M is an equivalence. As such we were interested in investigating the suitability of using OBO cross-products as a source of ternary compound mappings.

## 2.1 OBO cross-products

The OBO Foundry [10] is a collaborative initiative for establishing a set of principles for ontology development in the biomedical domain. Its goal is to support the creation of orthogonal interoperable reference ontologies. Ontologies that adhere to all principles are considered full members, whereas ontologies that adhere to only some of the principles are viewed as candidates. OBO cross-products were created to provide computable logical definitions for classes, by weaving together multiple OBO and OBO candidate ontologies. A large portion of OBO cross-products [11] are genus-differentia constructs of the form “an X is a G that D”, where X is the defined class, G is the superclass, and D corresponds to the characteristics that serve to differentiate instances of X from other instances of G specified using relations from the Relation Ontology (RO). These constructs typically involve two ontologies, one to which X and G belong, and another which provides classes to be used in D. These are represented in the OBO Format using *intersection\_of* tags, as depicted in Figure 1.

```
[Term]
id: GO:0000024
name: maltose biosynthetic process
intersection_of: GO:0009058 ! biosynthetic process
intersection_of: results_in_change_to CHEBI:17306 ! maltose
```

Fig. 1: Definition of a GO class in OBO with a cross-product involving GO and CHEBI classes.

However, there are also logical definitions that employ other constructs based exclusively on classes from other ontologies. For instance, many of the classes in the Human Phenotype Ontology have definitions that are composed of classes from the PATO and FMA ontologies (see Figure 2).

```
[Term]
id: HP:0000337 ! broad forehead
intersection_of: PATO:0000600 ! increased width
intersection_of: inheres_in FMA:63864 ! forehead
```

Fig. 2: Definition of a HP class in OBO with a cross-product involving PATO and FMA classes.

These kinds of cross-products can then be interpreted as a mapping between the class that is being defined and a complex class expression between two other classes.

Take as an example the class definition present in Figure 2. The class HP:0000337 labeled *broad forehead* is equivalent to an axiom obtained by relating the classes PATO:0000600 (*increased width*) and FMA:63864 (*forehead*) via an intersection qualified by an *inheres.in* relation. So, in this case, and going back to the ternary compound mapping definition: A is the HP class, B and C are PATO and FMA classes, R is an intersection, and M is equivalence.

## 2.2 Selecting cross-products collections to build alignments

We analyzed all thirty resources available at [obofoundry.org](http://obofoundry.org)<sup>1</sup>. We defined the following criteria to identify cross-products that are suitable to serve as a basis for a reference alignment:

- They represent a ternary relationship, whereby two classes are combined in a class expression that is equivalent to a third class
- Each of the classes belongs to a different ontology
- For each trio of ontologies, at least one hundred cross-products is available

The first two criteria filter out cross-products of the genus-differentia type and cross-products involving more than three classes. The third criterion ensures we obtain reference alignments of reasonable size, taking into consideration the dimension of the ontologies involved, and thus are useful to evaluate ternary ontology matching tasks.

These criteria resulted in a set of seven cross-products collections presented in Table 1.

Table 1: Selected cross-products collections

Source Ontology	Target Ontologies	Size
MP	PATO UBERON	1725
HP	PATO FMA	1519
MP	PATO CL	407
WBPhenotype	PATO GO	369
MP	PATO GO	354
FYPO	PATO GO	285
MP	PATO NBO	100

<sup>1</sup> <http://obofoundry.org/index.cgi?show=mappings>

### 2.3 Representing a ternary compound mapping

To create the alignments based on the cross-products collections we used EDOAL (Expressive Declarative Ontology Alignment Language) [12], since it allows the construction of entities from other entities using algebraic operators. To represent *intersection\_of* we employed a class expression with the *and* operator. The following represents one compound ternary mapping in EDOAL using as source the OBO cross-product in Figure 2:

```

<align:map>
  <align:Cell>
    <align:entity1>
      <edoal:Class rdf:about="http://purl.obolibrary.org/obo/HP_0000337"/>
    </align:entity1>
    <align:entity2>
      <edoal:Class>
        <edoal:and rdf:parseType="Collection">
          <edoal:Class rdf:about="http://purl.obolibrary.org/obo/PATO_0000600"/>
            <edoal:Class rdf:about="http://purl.obolibrary.org/obo/FMA_63864"/>
          </edoal:and>
        </edoal:Class>
      </align:entity2>
      <measure rdf:datatype="xsd:float">1.0</measure>
      <relation>=</relation>
    </align:Cell>
  </align:map>

```

## 3 Ontologies and Compound Alignments

The seven cross-products collections that fulfil our requirements are based on ten distinct ontologies, which are listed in Table 2. Notably, all seven collections share the Phenotypic Quality Ontology (PATO) as one of the target ontologies. This is unsurprising since all source ontologies are dedicated to representing phenotypes, i.e., the observable characteristics of an organism, and as such their classes can be logically defined by associating a given entity (e.g., *forehead*) with a specific characteristic (e.g., *increased width*). There has been a focused effort on the part of OBO ontologies to provide logical definitions in the form of cross-products for phenotype ontologies [13]. Cross-product creation was partially automated, but all cross-products are manually validated by at least two experts, and reasoners are employed to check for logical consistency.

Table 3 presents some statistics about the created alignments.

Table 2: Ontologies in cross-products collections

Acronym	Name	Classes	Domain
FYPO [14]	Fission Yeast Phenotype Ontology	6,176	Fission yeast phenotypes
HP [15]	Human Phenotype Ontology	10,593	Phenotypes of human hereditary and other diseases
MP [16]	Mammalian Phenotype Ontology	10,730	Mammalian phenotypes
NBO [17]	Neurobehavior Ontology	1,070	Behavior processes and normal and abnormal behavior phenotypes
WBPhenotype [18]	<i>C. elegans</i> Phenotype Vocabulary	2,185	<i>C. elegans</i> phenotypes
PATO [19]	Phenotypic Quality Ontology	2,444	Phenotypic qualities or properties
CL [20]	Cell Ontology	5,901	Cell types
FMA [21]	Foundational Model of Anatomy	83,283	Human anatomy
GO [22]	Gene Ontology	41,300	Gene product function
UBERON [23]	Uber Anatomy Ontology	12,808	Integrated cross-species anatomy

Information collected from BioPortal<sup>2</sup> in July 2014.

Table 3: Compound reference alignments composition

Alignment	Mappings	Unique Target 1 Classes	Unique Target 2 Classes
HP-PATO-FMA	1519	181	533
MP-PATO-UBERON	1725	210	679
MP-PATO-CL	407	33	171
MP-PATO-GO	354	60	205
MP-PATO-NBO	100	16	60
WBPhenotype-PATO-GO	369	59	254
FYPO-PATO-GO	285	21	166

## 4 Towards Ternary Ontology Matching

We explored the problem of ternary ontology matching, first by characterizing it, through the analysis of the mappings derived from the OBO cross-products, and then by conducting preliminary matching experiments.

### 4.1 Cross-Product Mapping Analysis

One of the principles accepted by the OBO Foundry is concerned with following naming conventions [24]. Two of these naming conventions are particularly tied to cross-products:

- **Recycle strings:** when creating compound names re-use strings as they occur in names of entities already defined elsewhere in this or in other ontologies.
- **Use genus-differentia style names:** apply modifiers to the head word of a class name to reflect the distinction from its parent class (e.g., *broad* forehead).

Given these characteristics we were interested in investigating the string similarity between the label of the source class and the union of the labels of the target classes. Furthermore, the importance of lexical based similarity for biomedical

ontology matching [25] and the high performance of string similarity in several ontology matching problems [26], make string similarity a logical first step towards matching these ontologies.

A simple computation of the exact similarity between the label of the source class and the concatenation of target labels produced the results in Table 4.

Table 4: Exact string similarity between source label and the concatenation of target labels.

Alignment	Exact Similarity Mappings	Total Mappings
HP-PATO-FMA	100	1519
FYPO-PATO-GO	4	285
MP-PATO-CL	1	407
MP-PATO-GO	18	354
MP-PATO-UBERON	76	1725
MP-PATO-NBO	0	100
WBPhenotype-PATO-GO	61	369

Very few of the mappings actually correspond to this compositional pattern, despite the OBO Foundry guidelines. However, in most cross-product mappings, the label of the source class shares at least one word with each of the target classes. Thus, we considered that a simple bag-of-words similarity would be the best approach to measure the overlap between the source and the union of the target labels.

We computed bag-of-words similarity by representing the label of each class as a set of words and joining the sets of the two target classes in a single set. Then we computed the intersection between the source and united target sets, and obtained a similarity score by dividing the cardinality of the intersection by the cardinality of the source set:

$$sim = \frac{|(S \cap (T_1 \cup T_2))|}{|S|} \quad (1)$$

We calculated these similarities for all mappings in each alignment. Figure 3 presents these results as percentage based histograms for each alignment. For most alignments, over 70% of the mappings share more than half the words.

## 4.2 Matching Experiments

In ontology matching, a common approach is to compute similarities between all classes of each of the ontologies. In standard binary matching problems, this leads to a quadratic search space, and so state-of-the-art ontology matching systems employ ‘anchor’-based strategies to increase efficiency [27, 28]. In ternary ontology matching, the search space is cubic, so matching even relatively small ontologies can pose efficiency problems. For instance, the search space in the MP-PATO-GO alignment is on the order of  $10^{12}$ . Moreover, the nature of the problem

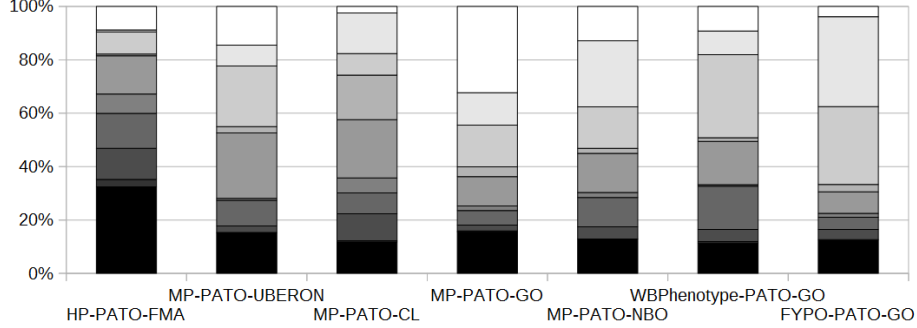


Fig. 3: **Distribution of label similarity for each generated alignment.** Each slice corresponds to a 0.1 interval of similarity. The height of each slice corresponds to the percentage of mappings whose label similarity falls within that interval.

does not lend itself to the use of full label matches, which are the most efficient ‘anchor’-based matching strategy. While theoretically possible, ‘anchor’-based word-matching [27] would have quadratic memory requirements, as we would need to compute all combinations of labels from both target ontologies.

The one aspect which facilitates efficiency is that we are only interested in capturing mappings where both target classes overlap in words with the source class. Thus, we can reduce the search space by first matching the source ontology to each of the target ontologies individually, using an ‘anchor’-based word-matching algorithm, and then matching only all pairs of target classes that map individually to the same source class. This was precisely the matching strategy we implemented to test ternary ontology matching.

Our implementation was based on the ontology matching system Agreement-MakerLight [27], and made use of its ‘anchor’-based WordMatcher, which measures similarity between two classes through a weighted Jaccard index between the words present in their labels.

To measure similarity between the source labels and merged target labels, we need to ensure that the target labels cover different portions of the source label, rather than sharing the same words. To this end, we employed a modified Jaccard index as a similarity metric:

$$WordMatch = \frac{|(S \cap (T_1 \cup T_2))| - |(T_1 \cap T_2)|}{|S \cup T_1 \cup T_2|} \quad (2)$$

This similarity metric accounts for the overlap between source and target labels, while penalizing words shared by both targets.

In spite of the reduced search space, we were not able to test this matching



strategy on trios that included the larger ontologies. We tested it in the MP-PATO-CL and MP-PATO-NBO alignments, obtaining recall values of 30 and 11% respectively, but precision values below 1%. These results are due to both the sheer dimension of the search space and the fact that the WordMatcher approach is unable to discriminate between a high number of candidate mappings that all share high similarities. Consider the following example:

Table 5: Example of indistinguishable mappings

Mapping Type	Source Class	Target 1 Class	Target 2 Class
correct	MP:0003545 increased alcohol consumption	PATO:0000912 increased rate	NBO:0000131 alcohol consumption
candidate	MP:0003545 increased alcohol consumption	PATO:0002361 increased tendency	NBO:0000131 alcohol consumption
candidate	MP:0003545 increased alcohol consumption	PATO:0002017 increased magnitude	NBO:0000131 alcohol consumption

There are 105 classes in PATO whose labels contain the word ‘increased’, of these only 29 contain more than two words. So even if we penalize non-matching words, there are 76 classes who give rise to the same similarity score. These results highlight some of the complexity behind compound alignments, even between ontologies that strive to follow the same naming conventions. We posit that to solve these issues, matching techniques would need some form of background knowledge or instances, to provide additional information able to discriminate between the candidate mappings.

## 5 Related Work

The most common way of evaluating an ontology matching system is through comparison of the alignment produced by the system with a reference alignment. This has been the standard method of evaluation conducted at the Ontology Alignment Evaluation Initiative [29]. Typically, reference alignments are manually constructed, however, the difficulty in creating these resources has motivated alternative methods of evaluation and reference creation.

One alternative method is to evaluate created mappings *a posteriori*. This approach has been used in the OAEI conference track [30], and over the years resulted in the construction of a reference alignment. However, the evaluation of complex correspondences is still manually conducted. In fact, establishing a reference alignment for complex correspondences is a complex and cumbersome task, so resorting to manual validation of generated mappings is needed [5]. However, this only allows identification of true positives and false positives (not false negatives), making it impossible to compute recall.

Employing external resources to support the creation of reference alignments has been used before in the biomedical domain, in the context of the Large

Biomedical Track of OAEI [31]. The UMLS Metathesaurus was used to automatically derive alignments between biomedical ontologies, which were then refined by employing automated repair methods and a few manual corrections. These alignments have been successfully used in recent OAEI editions, helping to answer the challenge of providing large-scale evaluation of ontology matching.

## 6 Conclusions

The field of ontology matching has been evolving in recent years to address some of its biggest challenges: efficiency, consistency, using background knowledge, user interaction, etc. One crucial aspect of fostering the development of new methods is the ability to evaluate performance. For instance, in the Large Biomedical Ontology track of OAEI, matching the track’s ontologies can result in logical inconsistencies. In 2012 only one system [28] was capable of adequately handling them, but in 2013 two other systems were also employing existing or novel repair techniques [32, 33]. It is clear that well-crafted benchmarks can drive innovation in a field.

With this work we have taken a first step in promoting the expansion of ontology matching systems towards more complex techniques that are capable of identifying more complicated relationships among multiple ontologies. Our preliminary experiments have shown that there are a number of issues in addressing this challenge, including the increase in matching space and the inherently more difficult-to-compute ternary mapping. Nevertheless, we look forward to a next-generation of ontology matching systems that go beyond equivalent 1:1 mappings and open up new application avenues.

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