

RDF2Vec-based Classification of Ontology Alignment Changes

Matthias Jurisch, Bodo Igler

RheinMain University of Applied Sciences
Department of Design – Computer Science – Media
Unter den Eichen 5
65195 Wiesbaden, Germany
matthias.jurisch@hs-rm.de, bodo.igler@hs-rm.de

Abstract. When ontologies cover overlapping topics, the overlap can be represented using ontology alignments. These alignments need to be continuously adapted to changing ontologies. Especially for large ontologies this is a costly task often consisting of manual work. Finding changes that do not lead to an adaption of the alignment can potentially make this process significantly easier. This work presents an approach to finding these changes based on RDF embeddings and common classification techniques. To examine the feasibility of this approach, an evaluation on a real-world dataset is presented. In this evaluation, the best classifiers reached a precision of 0.8.

Keywords: RDF Embedding, Change Classification, Ontology Alignment, Ontology Mapping, Mapping Adaption

1 Introduction

Finding alignments between ontologies, also known as ontology matching, is a non-trivial task and has been an active area of research over the last ten years. Several approaches in this area are based on the structure of the ontologies, logical axioms or lexical similarity [1]. However, once these alignments are found, they will not necessarily stay untouched forever. Especially when alignments connect large ontologies, adapting these alignments to changes is a work-intensive task. In the area of biomedical ontologies, some alignments contain around 6500 correspondences that might be affected by a change in one of the ontologies they connect. Given a change in the ontology, detecting which parts of the alignment are affected by the change and need to be adapted is not a trivial task that usually requires manual labour. The effort required for this task can be significantly reduced, if some changes can be excluded from it. However, it is usually not clear how to identify changes that do not affect the alignment.

In this paper, we propose an approach to this problem based on RDF embeddings and well-known classification techniques. The central aspect of this approach is to represent changed concepts by their RDF embedding and classify

whether an alignment statement nearby should be changed. To gain evidence if this approach works, we evaluate it using a dataset from the area of biomedical ontologies. On this dataset, our approach is able to identify changes affecting alignment statements with a precision of 0.8.

The remainder of this work is structured as follows: Section 2 discusses foundations of our work and related approaches. The general approach is presented in Section 3. Evaluation methodology, the dataset and results are shown in Section 4. Section 5 discusses the results of our evaluation, and advantages and disadvantages of our approach. A conclusion is given in Section 6.

2 Foundations and Related Work

An ontology alignment (sometimes also called ontology mapping) is a set of correspondences between entities in different ontologies [1]. To make it easier to reason about these alignments, we use the following formal definition in the style of [2] for ontology mappings: An alignment between two ontologies \mathcal{O}_1 and \mathcal{O}_2 is defined as

$$A_{\mathcal{O}_1, \mathcal{O}_2} = \{(c_1, c_2, semType) | c_1 \in \mathcal{O}_1, c_2 \in \mathcal{O}_2, semType \in \{\equiv, \leq, \geq\}\}$$

$A_{\mathcal{O}_1, \mathcal{O}_2}$ is the set of all *alignment statements*. To denote a change of an ontology over time, we use the prime symbol (e.g., a changed version of \mathcal{O} is denoted as \mathcal{O}'). The alignment adaption problem for two ontologies \mathcal{O}_1 and \mathcal{O}_2 connected by $A_{\mathcal{O}_1, \mathcal{O}_2}$ can then be stated as finding a new alignment $A'_{\mathcal{O}'_1, \mathcal{O}'_2}$, when \mathcal{O}_1 and \mathcal{O}_2 evolve to \mathcal{O}'_1 and \mathcal{O}'_2 .

In the area of ontology alignment adaption, several approaches are based on rules or rule-based dependency analysis. [5] is focussed on finding which changes are relevant to parts of the alignment using a dependency analysis. [10] proposed an *incremental approach* reacting to specific changes in database schemas based on rules. For each change pattern a specific modification for the mapping is defined. [12] proposed an approach that is based on a composition of alignments. A new alignment $A'_{\mathcal{O}'_1, \mathcal{O}'_2}$ is created by a *composition of the alignment* $A_{\mathcal{O}_1, \mathcal{O}_2}$ and $A^+_{\mathcal{O}_2, \mathcal{O}'_2}$, the alignment between \mathcal{O}_2 and \mathcal{O}'_2 . [2] have shown that these techniques can also be applied to ontologies. However, all of these approaches require a set of rules that need to be constructed by a domain expert and are not necessarily reusable for other domains. Also, these approaches are not able to identify which changes in the ontologies are prone to causing an alignment change.

The task of knowledge base completion shares some properties with the problem we address in this work. In that area, classifiers are given a subject and a predicate and try to predict an object [7]. Approaches like [11], [4] and [9] also use vector representations for prediction. However, this task does not take changes in the knowledge bases into account and is not applied to ontology alignments.

To our knowledge, no approach exists that predicts whether a given change has an impact on the alignment without using a detailed set of rules. This issue is at the core of our research.

3 Approach

Our general approach is based on the representation of changed resources using RDF embeddings, a representation of RDF nodes as vectors in a high-dimensional, dense vector space. RDF embeddings are generated using RDF2Vec [8], an approach based on random graph walks as input to Word2Vec [6]. The RDF2Vec-Model is trained on an RDF graph consisting of the ontologies \mathcal{O}_1 and \mathcal{O}_2 as well as the alignment $A_{\mathcal{O}_1, \mathcal{O}_2}$ as defined in section 2. With these embeddings, we train a classifier on whether a changed resource affected an alignment statement and use this classifier to predict whether other changes will affect the alignment. We define a changed resource to lead to an alignment change, if a changed alignment statement is within a distance of two in the RDF graph. This relatively small measure is used to make it easier to exclude certain regions from the search for affected statements. For the same reason, only changes that are close to an alignment axiom are regarded. The respective changes c are extracted using an extension of the Protégé plugin owl-diff¹. By comparing the parts of $A_{\mathcal{O}_1, \mathcal{O}_2}$ and $A'_{\mathcal{O}_1, \mathcal{O}_2}$ that are in the direct neighbourhood of c , it is possible to separate all changes into two groups: (1) changes that caused an alignment change in their neighbourhood and (2) changes that did not cause an alignment change in their neighbourhood and therefore did not affect the alignment.

Each changed resource is represented by the corresponding RDF2Vec vector. Hence, the input to the training of the classifier is a pair $(v(c), k)$ consisting of a vector $v(c)$ and a class k . k determines whether c caused a change in its direct neighbourhood. The task at hand is to correctly classify new vectors. To solve this problem, we use several common classification techniques: Regression, Naive Bayes, Tree-Based Algorithms as well as Support Vector Machines and Multilayer Perceptrons. Each algorithm is trained on one set of changes and evaluated on a different set.

4 Evaluation

The research questions behind our evaluation are the following:

1. Can RDF embeddings be used for change classification with an acceptable performance? This question tries to clarify, whether our approach is in general applicable to the problem at hand.
2. Which classifiers can be used for this problem? This question is used to identify the best classifiers for our problem.

4.1 Dataset

The dataset used to answer these research questions in our experiments is a real-word dataset from the domain of biomedical ontologies. It has been used

¹ <https://github.com/mhfj/owl-diff>

in several works that deal with alignment adaption, e.g., [3], [2]. The dataset comprises three ontologies: SNOMED-CT, the NCI-Thesaurus and FMA. For each ontology, yearly versions from 2009-2012 are available. Additionally, the dataset contains alignments extracted from the UMLS metathesaurus between the ontologies for each year. This dataset has been made publicly available² by the authors of [2].

For simplicity of our presentation, we will only present the alignment between the ontologies NCI and FMA in the version change from 2009 to 2010. In the formal notation introduced in Section 2, \mathcal{O}_1 and \mathcal{O}_2 refer to the ontologies NCI and FMA as of 2009 and \mathcal{O}'_1 and \mathcal{O}'_2 as of 2010, respectively. The alignment from 2009 is denoted by $A_{\mathcal{O}_1, \mathcal{O}_2}$ and the version from 2010 by $A'_{\mathcal{O}'_1, \mathcal{O}'_2}$.

From 2009 to 2010, 924 changes are near alignment statements of which 47% require an adaption. These changes are used as a training set. The test set consists of the changes from 2010 to 2011. This set contains 785 changes near alignment statements, of which 36% lead to an alignment adaption.

4.2 Methodology

To generate RDF embeddings, the code from RDF2Vec [8] was used. The embeddings were trained using the skip gram model, with 500 dimensions used for the embeddings and random walks of length 8, as this was identified as the best-performing variant in [8]. An overview regarding classification methods used on these embeddings is given in Table 1. Standard scikit³ implementations are used for the classification process. The classifiers are trained on changes from 2009-2010 and validated on changes from 2010-2011 of the dataset described in Section 4.1. The performance of different classification techniques is evaluated based on *f1-measure*, *accuracy*, *precision* and *recall*.

Table 1. Classifiers

| Category | Method |
|-------------------------|---|
| Regression | Logistic Regression (LR) |
| Naive Bayes | Gaussian Naive Bayes (NB) |
| Nearest Neighbour | KNN |
| Tree-Based Algorithms | CART, Random Forest |
| Support Vector Machines | RBF-Kernel, Linear Kernel |
| Multilayer Perceptron | MLP hidden-layer-size: 250; 250,250; 500; 500,500 |

² https://dbs.uni-leipzig.de/de/research/projects/evolution_of_ontologies_and_mappings/ontology_mapping_adaption

³ <http://scikit-learn.org/stable/>

4.3 Results

The results of the described process are displayed in Table 2. Only changes close to the alignment were included in this evaluation, since it would otherwise be very easy to achieve accuracy values above 95%. Results for MLP did not vary based on the structure of the hidden layers, so one row represents all MLP results. All algorithms show a very similar performance regarding the evaluated metrics. The highest achieved precision is 0.81, which can be reached using MLP and linear SVM classification. These methods also reach the highest f1-measures of 0.75. Accuracy of all classifiers is only marginally higher than what can be achieved using random guessing, given the distribution of classes in the test set.

Table 2. Classification Results

| | <i>f1-measure</i> | <i>accuracy</i> | <i>precision</i> | <i>recall</i> |
|--------------|-------------------|-----------------|------------------|---------------|
| LR | 0.74 | 0.67 | 0.80 | 0.69 |
| NB | 0.67 | 0.58 | 0.73 | 0.62 |
| KNN | 0.71 | 0.62 | 0.75 | 0.69 |
| CART | 0.73 | 0.65 | 0.80 | 0.68 |
| RandomForest | 0.75 | 0.67 | 0.80 | 0.70 |
| SVM rbf | 0.74 | 0.65 | 0.77 | 0.71 |
| SVM linear | 0.75 | 0.67 | 0.81 | 0.70 |
| MLP | 0.75 | 0.68 | 0.81 | 0.70 |

5 Discussion

The results presented in section 4.3 give us some evidence on our first research question: Using RDF embeddings to represent changes seems to be a promising approach to the mapping adaption problem, as we can see a precision around 0.8. In general, several classification approaches show a similar performance. This precision can be achieved, although the approach uses no information regarding the nature of changes, e.g., the algorithm can not distinguish the correction of typos from major, structural changes.

An important advantage of this approach is that no sophisticated change model that is adapted to the domain is required. Approaches like [2] require a rule-base that needs to be constructed from a detailed understanding of typical changes in the domain the ontologies describe. Hence, the author of these rules needs to be an expert in ontology engineering as well as the application domain. Also, these rules need to be constantly adapted to evolving domains, whereas an RDF-embedding based approach could learn new patterns autonomously. However, to demonstrate these advantages, it is still required to show that this approach is also applicable to other data sets and different application domains.

6 Conclusion and Outlook

In this work, we presented an approach to ontology alignment adaption based on RDF embeddings and common classification techniques. An evaluation on a dataset from the biomedical domain provided some evidence, that the approach is feasible. On the dataset, best-performing classifiers had a precision of 0.8.

As future work, several extensions are possible: Further evaluations could be performed on different datasets. Also, a combination of this approach with existing mapping adaption approaches could be examined. Change types could be used as another input to the classification process to improve classification accuracy. Another aspect for future work is to determine, when embeddings need to be updated, since embeddings will become outdated when ontologies change.

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