Matching Large Biomedical Ontologies Using Symbolic Regression

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ABSTRACT

The problem of ontology matching consists of finding the semantic correspondences between two ontologies that, although belonging to the same domain, have been developed separately. Matching methods are of great importance since they allow us to find the pivot points from which an automatic data integration process can be established. Unlike the most recent developments based on deep learning, this study presents our research on the development of new methods for ontology matching that are accurate and interpretable at the same time. For this purpose, we rely on a symbolic regression model specifically trained to find the mathematical expression that can solve the ground truth accurately, with the possibility of being understood by a human operator and forcing the processor to consume as little energy as possible. The experimental evaluation results show that our approach seems to be promising.

CCS CONCEPTS

• **Information systems** → **Expert systems**; Recommender systems; • **Information Systems** → *Data Mining*.

KEYWORDS

Information Integration, Ontology Matching, Similarity Measures

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1 INTRODUCTION

Ontology matching is a field for finding semantic correspondences between ontologies belonging to the same domain but developed separately. Despite its importance in many computer-related disciplines, several problems are currently associated with systems for automatically matching ontologies. For example, the existing program interfaces are not very attractive. The existing matching systems do not allow the discovery of complex correspondences. Most of the existing semantic similarity measures to discover similar entities across ontologies cannot be aggregated easily.

In recent years, we have witnessed an explosion in the number of new techniques and tools for ontology matching, filling these gaps to overcome these problems. These techniques and tools have been a leap in quality compared to the state-of-the-art because they have solved many issues related to the accuracy, recall, aggregation, speed of computation, etc. However, there are still some open issues to solve the problem almost definitively. In this paper, we address one of these open issues: interpretability, i.e., the potential ability of a human operator to understand a matching model that has been derived analytically using some computational learning technique.

Biomedical ontology matching, sometimes also called biomedical ontology alignment, consists of finding the semantic correspondences between entities belonging to two ontologies from the biomedical domain that have been developed independently by different teams. One of the main characteristics of this domain is that biomedical ontologies are usually considered large when most state-of-the-art approaches are merely applicable for small-scale ontologies. This usually means that the effectiveness of the existing approaches decreases for large ontologies. This makes our challenge slightly different from the usual one, matching many small ontologies (called holistic matching). Furthermore, there is an additional problem when determining these approaches because reference correspondences are unknown in advance, so domain experts must assess samples of the mappings proposed and returned results.

Due to the decentralized nature of biomedical research, the problem is that there usually exist multiple ontologies from overlapped application domains or even within the same domain. In order to establish interoperability between biomedical applications that use different but related ontologies, ontology matching has been proposed as an effective way of handling the semantic heterogeneity problem. It is typically valuable for some data management applications, such as information integration and merging as well

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as distributed query processing. Some ontology matching techniques based on machine learning have recently obtained remarkable results in the biomedical domain. However, the problem is that machine learning methods rely heavily on the availability of high-quality labeled data.

Moreover, if we look exclusively at the latest techniques based on deep learning, we find another problem: The solutions often behave like black boxes that users find difficult to trust. The reason is that solutions based on deep neural networks can accept input and provide an output but often do not allow the human operator to understand what happened inside the model before arriving at that output. This is a severely limiting factor that hinders automatic measures for ontology alignment in the biomedical field.

Today, many applications require matching biomedical ontologies; we have focused on addressing this challenge by using highly interpretable matching methods based on the concept of symbolic regression. In this way, the significant contributions of this work can be summarized as follows:

(1) We propose, for the first time, a method to match large biomedical ontologies based on the concept of symbolic regression intended to facilitate the interpretability of the resulting matching models.
(2) We empirically evaluate this new method using the most popular benchmark datasets in the biomedical domain and offer a comparison with the most prominent ontology matching tools.

The rest of this work is structured in the following way: Section 2 describes the state-of-the-art regarding ontology matching in the biomedical field. Section 3 presents our technical contribution. Section 4 presents the results we have achieved after performing several experiments and compares our results with other prominent approaches. Finally, we remark on the strengths and flaws of our proposal and discuss the future work.

2 STATE-OF-THE-ART

One of the earliest studies to formalize this problem was [13], which addressed how ontology matching systems may be created through a trade-off between precision and recall. These authors were the first to propose that instead of using an ontology matching algorithm, machine learning models should be used to generate the most efficient and effective ensemble of matchers. From this seminal work, the study turned to the proposal of machine learning methods to aggregate the fundamental matchers, with GAOM [23] and GOAL [15, 16] being the first studies being able to construct the ensemble using genetic algorithms. The fundamental notion was that it might optimize the precision, recall, or combination of the two. In [17], a survey on ontology matching was presented with emphasis on the aggregation methods used by the different proposals existing to date, as well as the significant differences between the techniques for matcher combination, matcher self-tuning, and meta-matching.

It is important to remark that dealing with large ontologies is a problem that entails a higher complexity than usual. The many homonyms and relationships that only apply in narrow subject domains will lead to many incorrect matches. For general use cases, methods based on the exploitation of embeddings can yield better results. Nowadays, one of the most well-known approaches using embeddings is that of Kolyvakis et al. [11]. The authors propose that ontological term vectors based on information derived from textual corpora and other resources be used to solve the problem. Wu et al. have also lately used Siamese networks to outperform the state-of-the-art in specific instances [24]. Both approaches, however, are based on deep learning. This implies that they have significant interpretability issues.

One of the areas where the effective and efficient use of ontologies can significantly impact is the biological field. Biomedical ontologies are a rich source of information that can help developers create applications for biomedical data annotation, knowledge discovery, decision making, and data interoperability. In this scenario, mappings between the entities corresponding to each ontology are critical for interoperability between data sources. However, semantic heterogeneity is a critical issue that frequently inhibits the construction of these mappings. As a result, several solutions have been presented [7, 9, 12, 21, 25].

Regarding the sources to be used, some biomedical ontologies such as SNOMED [5], the National Cancer Institute Thesaurus (NCI) [3], and the Foundational Model of Anatomy (FMA) [19] have become quite popular and are often used in various solutions and systems. However, to date, most proposals for matching biomedical ontologies have focused mainly on feature engineering. Features include terminological, structural, extensional (instances of a given concept), and external resources. Therefore, the quality of the results has been restricted to small scenarios [10]. There have been several attempts to establish the biomedical ontology matching problem as a binary classification problem, i.e., a classifier could be trained with a sample of positive and negative examples provided by that user to identify the cases once it is put into production correctly. However, the results cannot yet be considered optimal. In recent times, deep learning-based solutions seem to have succeeded in overcoming almost all traditional limitations, including outstanding performance in terms of accuracy in a wide range of scenarios [11, 24]. This is due to a large number of homonyms and associations that only apply to specific subject domains, which will result in a large number of false matches. It is widely assumed that in most applications, embedding-based matching will produce better results. However, there are still some gaps, such as the interpretability of the resulting model to be addressed.

This work presents the problem as a challenge of getting a symbolic mathematical expression to identify the relationship between defined input and output variables. The mathematical expression is allowed to be flexible without being restricted to a particular structure. In our case, the output is the ontology matching score associated with a pair of entities, while the input variables are values coming from highly interpretable basic matching algorithms already proposed. In this way, the search space of candidate expressions is really huge. Therefore, it is a much more difficult task than other kinds of regression, such as linear or polynomial regression. The great advantage is that the learned model is a mathematical equation that can be examined and interpreted in the context of the given situation. That resulting equation is not only chosen to fit the input data but provides a functional explanation of the resulting model.

3 MATCHING ONTOLOGIES USING SYMBOLIC REGRESSION

One of the most well-known applications of ontology technologies is the domain of life sciences. Ontologies are regulated terminologies that allow people and machines to understand the meaning of data legibly. In this way, one of the primary goals of biomedical ontologies is to express classes of items relevant to the ontology's development context. However, in addition to the names associated with these classes, the relationships between the various classes are also meaningful. Let us see some definitions of our approach.

3.1 Definitions and problem formulation

Definition 1 (Similarity Function). *A similarity function sf is a function* $sf : \mu_1 \times \mu_2 \mapsto R$ *that associates the similarity of two input pieces of information* μ_1 *and* μ_2 *to a similarity score* $sc \in \Re$ *in the range [0, 1].*

So that a score of 0 stands for absolute inequality and 1 for equality of the pieces of information μ_1 and μ_2 being compared.

Definition 2 (Ontology Matching). *An ontology matching om is a function* $om : O_1 \times O_2 \overset{sm}{\rightarrow} A$ *that associates two input ontologies* O_1 *and* O_2 *to an alignment A using a similarity function sf.*

Definition 3 (Ontology Alignment). *An ontology alignment oa is a set* $\{t, MD\}$*, whereby t is a set of tuples in the form* $\{(id, e, e', n, R)\}$*, being id a unique identifier, e and* e' *are entities belonging to two different ontologies, R is the relation of correspondence between these entities, and n is a real number between 0 and 1 that representing the plausibility that R may be true. The entities that can be related are the classes or the relationships of the ontologies. Furthermore, MD is some metadata related to the process for statistical purposes.*

Definition 4 (Alignment Evaluation). *An alignment evaluation ae is a function* $ae : A \times A_R \mapsto precision \in \Re \in [0, 1] \times recall \in \Re \in [0, 1]$ *that associates an alignment A and a reference* A_R *to two real numbers stating the precision, recall of A in relation to* A_R*.*

Definition 5 (Meta-Matching Function). *A Meta-Matching Function mmf is a function* $mmf : SC \mapsto \Re$ *that defines how previously calculated similarity score* $sc_i \in SC$*. The result is an optimized similarity score* $sc_o \in \Re$. We call optimized similarity score to the best possible similarity score.

In our case, the meta-matching function will be built using symbolic regression via genetic programming. Genetic programming uses evolutionary strategies to search for one good model from a vast space of solutions representing all the mathematical expressions dealing with the input data. Therefore, evolutionary strategies are a learning algorithm that combines two good individuals to create a superior individual. Evolutionary strategies are helpful because they do not use a straightforward optimization approach, allowing for a wide range of outcomes. Furthermore, the resulting model frequently comes up with innovative solutions that provide new insights into the problem.

3.2 Symbolic Regression

Symbolic regression is a kind of regression analysis in which the model that best fits a given input dataset is found by searching the entire space of all conceivable mathematical expressions. Symbolic regression has already been utilized to solve specific function identification and learning problems in the past. This is primarily owing to the concept of Abstract Syntax Tree (AST), which allows identifying any linear or non-linear function from previously solved cases.

Furthermore, the resulting model is immediately exportable in the form of an algorithm to several programming languages, making it easier for a human operator to comprehend and transfer to other situations of a similar nature, as we have already shown in [18]. This AST can evolve thanks to an underlying evolutionary strategy. The final result can be calculated by evaluating each node and then performing the parent node operation on the child nodes.

Our goal is for AST to evolve to accommodate an expression that perfectly fits the input-output pairs provided as a training dataset to use that mathematical expression to validate it over a test dataset. One of the additional advantages of symbolic regression models is that they also allow us to optimize the precedence of operators, which gives even more computing power to the model. Also, not letting the tree grow too much helps us avoid over-fitting problems. This is mainly since simple models behave better in terms of generalization of solutions than complex ones.

To do that, our goal is to aggregate existing matching methods strategically. Aggregation methods are prevalent in various areas of computing and are often used in production environments, as they allow to blur the errors that a method makes between a set of methods that usually work well most of the time, e.g., [14, 20, 22]. In rare cases where all the methods might simultaneously make the same mistake, the aggregation methods lose their effectiveness. In this way, some of the most common aggregation operators are the arithmetical mean, the median, and the geometric mean. However, their aggregation strategy is short-sighted since it cannot model an adequate interaction between the input similarity measures.

Last but not least, we know that there are three levels of model interpretability: Application-level (only an expert can understand the model), User level (anyone should be able to understand the model), Functional level (the model is expressed as a function). Our approach is the first, to the best of our knowledge, to reach the functional level [6].

4 EXPERIMENTAL EVALUATION

In this section, we present the empirical study to which we have subjected our approach. We have divided the section into the following subsections: We first describe the nature of the datasets we are working with. Secondly, we explain the metrics that will be used to assess the results obtained. Third, we report the configuration we have used to obtain the results. Fourth, we provide the raw results obtained by our approach and rigorous comparison with state-of-the-art. Fifth, we describe how our approach can model a trade-off between accuracy and interpretability properly. Furthermore, finally, we discuss the highlights of the whole empirical study.

4.1 Datasets

The datasets used in ontology matching are generally based on large-scale open-source data sources. In this work, we have focused on ontology from the biomedical domain as already reported by Kolyvakis et al. [11]. We consider here the foundational Model of Anatomy (FMA), which represents the phenotypic structure of the human body [19]. The Adult Mouse Anatomical Dictionary (MA) represents the anatomy of an adult mouse [8]. The NCI Thesaurus (NCI) provides standard terminology for cancer [3] and its anatomy subdomain describe naturally occurring human biological structures. Furthermore, finally, the SNOMED collection (SNOMED) represents medical nomenclature to be used in clinical reports [5].

4.2 Evaluation criteria

To evaluate the results of our empirical study, we will use the classical criteria of an information retrieval problem, as do most studies in this context. For this, we will use the traditional metrics based on precision, recall, and f-measure. Precision is the fraction of retrieved mappings that are relevant to the query. The recall is the fraction of the relevant mappings that are successfully retrieved. F-measure combines precision and recall is the harmonic mean of precision and recall. It is widely assumed that accuracy can be optimized at the expense of recall and vice versa. For this reason, it is convenient to report the two measures together.

4.3 Empirical study

To assess the performance of our approach, we also analyzed some of the best proposals in this context. This list is based on and expands the compilation made by [24]. In fact, we collect all its variants based on Deep Learning, in addition to the following solutions: AML [7], DOME [21], FCAMapKG [25], LogMapBio[9], and POMAP++ [12]. In this way, Table 1 shows the results for the MA-NCI that contains 1489 positives from 9 million possible correspondences. Please note that the ground truth for this experiment is based on the work of Bodenreider et al. [2].

Table 2 shows the results for the benchmark FMA-NCI. The ground truth for this experiment is based on the UMLS Metathesaurus [1] and it contains 2504 positive cases from 24 million possible correspondences.

Table 3 shows the results for the FMA-SNOMED benchmark dataset. Once again, the ground truth for this experiment is based on the UMLS Metathesaurus [1]. It has 7774 positives from 136 million possible correspondences.

4.4 Modeling trade-off between accuracy and interpretability

As a demonstration of what is possible in our solution but not possible in others, we model a trade-off between accuracy and interpretability. Since both are considered orthogonal objectives, we can formulate the problem as a bi-objective optimization. In such a problem, we look for the Pareto non-dominated solution front that solves the problem in the best way (e.g., maximum f-measure and interpretability simultaneously). In our case, interpretability is given by a smaller number of items in the resulting AST (and thus the equation). By non-dominated solutions, we mean solutions that can no longer improve one of the two objectives except at the expense of the other. All the solution fronts have been obtained with the multi-objective NSGA-II [4] algorithm which is considered a reference in the field of optimization. In this way, Figure 1 shows us the Pareto front of non-dominated solutions obtained when solving the MA-NCI dataset.

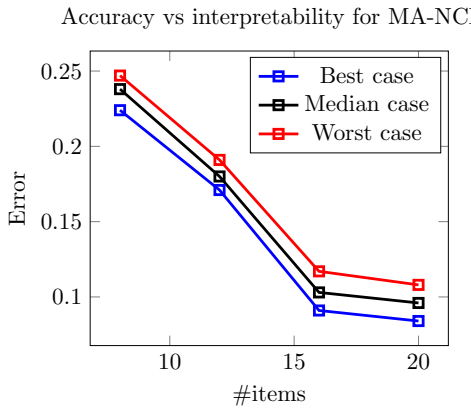

Figure 1: Pareto front of non-dominated solutions obtained when solving the MA-NCI dataset

Figure 2 shows us the Pareto front of non-dominated solutions obtained when solving the FMA-NCI dataset.

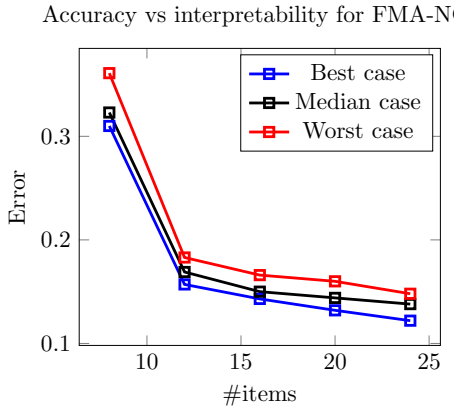

Figure 2: Pareto front of non-dominated solutions obtained when solving the FMA-NCI dataset

Finally, Figure 3 shows us the Pareto front of non-dominated solutions obtained when solving the FMA-SNOMED dataset.

These experiments make it possible to appreciate a great novelty compared to existing solutions to represent a trade-off between accuracy and interpretability. This means that human operators can have a list of options in front of them at all times, allowing them to choose the configuration that best matches the problem at hand. This is the first time this option has been made available in this domain to the best of our knowledge. The reason for this is that, whereas matching approaches have provided users with a trade-off between precision and recall, we are unaware of any

Method	precision	recall	f-measure	Interpretability
OM-TD (TF-IDF)	0.900	0.648	0.785	No
OM-TD (LSTM)	0.968	0.704	0.815	No
OM-TD (TBERT)	0.977	0.702	0.817	No
OM (LSTM + SGAT)	0.975	0.717	0.826	No
OM (TBERT + GraphSAGE)	0.954	0.529	0.681	No
OM (TBERT + TransE)	0.890	0.502	0.642	No
OM (DAEOM)	0.981	0.748	0.849	No
DOME	0.993	0.615	0.760	No
AML	0.950	0.936	0.943	Application Level
FCAMapKG	0.996	0.631	0.772	Application Level
LogMapBio	0.872	0.925	0.898	Application Level
POMAP++	0.919	0.877	0.897	Application Level
Our approach	**0.962**	**0.873**	**0.916**	**Functional Level**

Table 1: Results obtained for the MA-NCI

Method	precision	recall	f-measure	Interpretability
OM-TD (TF-IDF)	0.969	0.734	0.835	No
OM-TD (LSTM)	0.958	0.871	0.912	No
OM-TD (TBERT)	0.966	0.878	0.920	No
OM (LSTM + SGAT)	0.971	0.879	0.923	No
OM (TBERT + GraphSAGE)	0.981	0.738	0.843	No
OM (TBERT + TransE)	0.961	0.558	0.706	No
OM (DAEOM)	0.989	0.888	0.936	No
DOME	0.985	0.764	0.861	No
AML	0.958	0.910	0.933	Application Level
FCAMapKG	0.967	0.817	0.886	Application Level
LogMapBio	0.919	0.912	0.915	Application Level
POMAP++	0.979	0.814	0.889	Application Level
Our approach	**0.907**	**0.848**	**0.878**	**Functional Level**

Table 2: Results obtained for the FMA-NCI

Method	precision	recall	f-measure	Interpretability
OM-TD (TF-IDF)	0.941	0.613	0.742	No
OM-TD (LSTM)	0.972	0.687	0.805	No
OM-TD (TBERT)	0.977	0.715	0.826	No
OM (LSTM + SGAT)	0.981	0.732	0.838	No
OM (TBERT + GraphSAGE)	0.913	0.677	0.777	No
OM (TBERT + TransE)	0.722	0.506	0.595	No
OM (DAEOM)	0.990	0.791	0.879	No
DOME	0.988	0.198	0.330	No
AML	0.923	0.762	0.835	Application Level
FCAMapKG	0.973	0.222	0.362	Application Level
LogMapBio	0.931	0.703	0.801	Application Level
POMAP++	0.906	0.260	0.404	Application Level
Our approach	**0.907**	**0.770**	**0.832**	**Functional Level**

Table 3: Results obtained for the FMA-SNOMED

existing methodology to represent a trade-off between f-measure and interpretability.

5 CONCLUSIONS AND FUTURE WORK

In a time where methods for big data analysis are essential players in biomedical research, the need for people to trust the data-driven systems they use for their daily operations is crucial. However, in recent times, the field of ontology matching, particularly biomedical ontology matching, has been involved in a race to improve accuracy over and over again. This issue has caused to pay little attention to the interpretability of the increasingly accurate solutions.

When it comes to matching biomedical ontologies, our method produces acceptable results. Moreover, new matcher combinations can be tested based on the results. Even though only a few have been chosen, our method allows us to aggregate any matcher without degrading performance. In this way, it may make biological data sharing and integration across heterogeneous sources easier and accelerate the creation of biomedical data repositories applications. Future work, aside from looking for ways to improve accuracy, interpretability, and model good mixes, also needs to design novel solutions tailored to the user's preferences. It is widely assumed that more research in this area is required before the idea of replicating

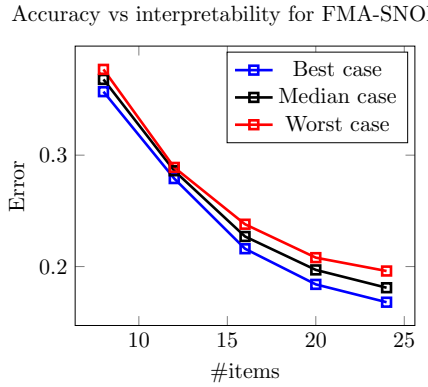

Figure 3: Pareto front of non-dominated solutions obtained when solving the FMA-SNOMED dataset

the human operator when dealing with semantic relations becomes a reality.

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