Why Settle for Just One? Extending $\mathcal{EL}^{++}$ Ontology Embeddings with Many-to-Many Relationships

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1 INTRODUCTION
The availability of data along with the computational power has led to the rise of deep learning which has become an important tool in various fields like computer vision and natural language processing. Despite the huge success, artificial neural networks have not been able to perform well on reasoning and logical tasks. They suffer from issues such as explainability and robustness. Knowledge Graphs [9] and ontologies [8] are structural knowledge bases that capture the relationship between different entities making them suitable for reasoning tasks. Unfortunately they are not ideal for real time usage as reasoning time, especially on complex and large ontologies could have worst-case exponential time complexity. Hence there is a trade-off between expressivity and complexity of such reasoners.

Knowledge Graph (KG) embeddings are an effort to combine the knowledge present in the Knowledge Graphs with the generalisation capability of the neural networks [18]. KG embeddings learn embedding functions that map the entities of Knowledge Graphs to vector space. Different Learning methods for such embeddings have been proposed [3, 12, 15, 20–22] that try to preserve various properties of these knowledge bases. In case of ontologies, they help create approximate reasoners which could reason on complex ontologies while having low time complexity.

Description logics [10] are a family of knowledge representation languages that provide the formal underpinning for Web Ontology Language (OWL). OWL 2, which is the most recent version of OWL, is used to build ontologies. They provide the schema information for the knowledge captured in KGs.

Most of the KG embeddings fail to consider the underlying constraints and characteristics of the ontologies. Hence, reasoning tasks do not perform well on such embeddings of ontologies. In order to tackle this issue, Kulmanov et al. [11] proposed EL Embeddings (EmEL) that incorporate the geometric structure of $\mathcal{EL}^{++}$ description logic ontologies into the embeddings. Mondal et al. [14] later added role oriented $\mathcal{EL}^{++}$ constructs into the embeddings through their proposed EmEL$^{++}$ method. While these methods have provided a new technique to perform reasoning tasks on the ontologies, they have a fundamental issue that restricts their performance on $\mathcal{EL}^{++}$ ontologies and restricts them from being used in more complex description logic based ontologies such as $SROIQ$, which is the basis for OWL 2 DL, a fragment of OWL 2. We provide a simple
and effective way to convert the embedding functions such that the roles (relation equivalent in ontologies) can be considered as many-to-many instead of one-to-one functions as is in the case of EmEl. This is significant as most of the roles in ontologies connect a class to multiple classes. For example, the fatherOf role can connect an individual to multiple individuals if he is the father of all of them. This issue becomes more important when we try to move to complex description logics like SROIQ which has properties such as cardinality that depend on many-to-many roles.

Contributions: (1) We provide a simple method to incorporate many-to-many roles in translation based embeddings like TransE [3]. (2) We show how the method could be used to modify the ontological embedding EmEl [11]. (3) We demonstrate the effectiveness of the method on three publicly available ontologies. (4) Our work provides a foundation for work on complex DL reasoners.

2 RELATED WORK

Node2Vec [7] used the concept of representing facts as triples of the form (h,r,t) which became a standard for various other models. Similarity based scoring functions were used in this work. In order to capture the underlying properties of the knowledge bases TransE [3] considered the relations in a KG as a translation operator over the entities and used distance based scoring functions. TransH [21] further allowed the relations to be many-to-many and reflexive by modelling the relations as a hyperplane in the vector space. DistMult [22] on the other hand used matrix factorisation to relate various entities. Existing works on ontology embedding such as Onto2vec [19] focuses on using word2vec as an underlying model. While the work focuses on encoding the entities and relations, it is unable to handle complex relations in an ontology.

[6] provide neuro-symbolic deep deductive reasoners for E.L++ DL and first-order logic. [13] pointed out that geometric models are a better way to learn embeddings for ontologies. The simplicity of the translation based models for KG embeddings [3, 21, 22] to measure the correctness of a fact as a distance between entities after being translated by the relation made them popular. EmEl [11] and EmEl++ [14] used this translation technique to create embeddings for ontologies which preserve their underlying structures and characteristics. In order to accomplish it, the models use geometric models to learn embeddings. The classes are considered to be n-balls in an n-dimensional space which are translated by the relation vectors to the n-ball of the corresponding class of the fact. This geometric structure provides a way to incorporate various structural properties of an ontology eg. subclass properties. However, like TransE, these models too restrict their triplets to a one-to-one mapping. Not only do these restrictions affect the performance of these models on E.L++ ontologies but also restrict them from being used in more complex description logics such as SROIQ.

3 BACKGROUND ON ONTOLOGY EMBEDDINGS

Kulmanov et al. [11] introduced the concept of incorporating geometric structure of ontologies into the embeddings. They proposed embeddings for the E.L++ description logic (EmEL) that captures the underlying structures and characteristics of the ontology by treating ontology classes as n-balls in n-dimensional space. These n-balls are represented by a center which is a n-dimensional vector and a radius which is a scalar. The relations in the ontology are considered as n-dimensional vectors which are used to translate the class from one point in the space to another. The center and the radius of each class (n-ball), along with the relations can be learnt over multiple iterations. They make up the embeddings for the ontology. Figure 1(a) and Figure 1(b) show the geometric representation of classes and relations in 2-dimensional space.

Hence, they define a geometric ontology embedding \( \eta \) as a pair \((f_q, r_q)\) of functions that map classes and relations in ontology \( O \) into \( \mathbb{R}^n \). Thus \( f_q : C \cup R \rightarrow \mathbb{R}^n \) and \( r_q : C \rightarrow \mathbb{R} \). Here \( C \) is a class and \( R \) is a relation and \( O \) is defined as \((C, R, \subseteq, ax)\) where \( \subseteq \) is individual symbols, \( C \) is set of class symbols, \( \mathbb{R}^n \) is set of relation symbols and \( ax \) are axioms (facts).

Basically, \( f_q(c) \) represents center of \( C \), \( r_q(c) \) represents radius of \( C \) and \( f_q(r) \) represents vector of \( R \).

Each axiom, \( ax \), is transformed into its equivalent normal form using a set of conversion rules from [2]. These rules help transform the set of axioms in the ontology into one of four forms without any loss of information. These are (1) Subclass axiom: \( C \subseteq D \) (2) Intersection axiom: \( C \cap D \subseteq E \) (3) Existential restriction (right-hand side): \( \exists R.D \subseteq E \) and (4) Existentil restriction (left-hand side): \( \exists C \subseteq D \) where \( C, D, E \subseteq C \) and \( D, E \subseteq \mathbb{R} \).

EmEl formulates a loss function for each of the four normal forms in order to preserve the semantics of \( E.L++ \) in the embeddings. The loss functions are as follows.

\[
\text{loss}_{C \subseteq D}(c, d) = \max(0, \| f_q(c) - f_q(d) \| + r_q(c) - r_q(d) - \gamma) + \| f_q(c) \| - 1) + \| f_q(d) \| - 1 \quad (1)
\]

In Eqn 1, we try to preserve the subclass property of the entities. Here the euclidean distance between the centers of \( C \) and \( D \) should be less than the difference between the radius of \( C \) and \( D \). Once this is achieved, we ensure that the n-ball representing \( D \) is bigger than that of \( C \) and that n-ball of \( C \) lies completely inside \( D \). Here \( \gamma \) is a hyperparameter called margin. \( \| f_q(c) \| - 1\) + \( \| f_q(d) \| - 1\) ensures that the n-balls lie in the unity sphere.

\[
\text{loss}_{C \cap D \subseteq E}(c, d, e) = \max(0, \| f_q(c) - f_q(d) \| - r_q(c) - r_q(d) - \gamma) + \max(0, \| f_q(e) - f_q(c) \| - r_q(c) - \gamma) + \max(0, \| f_q(d) - f_q(e) \| - r_q(d) - \gamma) + \| f_q(c) \| - 1) + \| f_q(d) \| - 1) + \| f_q(e) \| - 1) \quad (2)
\]

In Eqn 2, we incorporate the intersection property. The first term ensures that \( C \) and \( D \) are not disjoint sets. While second and third terms force the center of \( E \) to lie in the intersection of \( D \).

\[
\text{loss}_{\exists R.D \subseteq E}(c, d, r) = \max(0, \| f_q(c) - f_q(r) \| - r_q(c) - r_q(d) - \gamma) + \| f_q(c) \| - 1) + \| f_q(d) \| - 1) \quad (3)
\]

\[
\text{loss}_{\exists R.C \subseteq D}(c, d, r) = \max(0, \| f_q(c) - f_q(r) \| - r_q(c) - r_q(d) - \gamma) + \| f_q(c) \| - 1) + \| f_q(d) \| - 1) \quad (4)
\]

Eqn 3 and Eqn 4 describe the loss function for the third and fourth normal forms respectively. Every point that lies within an
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Every relation has its own $\sigma$ which is learnt during training. In order to avoid $\sigma$ from becoming infinite, we keep the absolute value of $\sigma$ as a loss component for regularisation. Figure 1(c) shows a visual representation of $\text{EmEl(var)}$. Hence, the definition of the geometric ontology embedding $\eta$ now becomes a tuple $(f_\eta, r_\eta, \sigma_\eta)$ of functions that map classes and relations in ontology $O$ into $\mathbb{R}^n$, where $f_\eta : C \cup R \mapsto \mathbb{R}^n$, $r_\eta : C \mapsto \mathbb{R}$ and $\sigma_\eta : R \mapsto \mathbb{R}$. The modified loss functions are provided in Eqn 7 and Eqn 8. Note that the loss function for other normal forms remain the same as in $\text{EmEl++}$. Baselines: We use the following publicly available ontologies of varying sizes.

1. GALEN [17] captures clinical information. It consists of 84,537 axioms with 1,010 relations and 24,353 classes.
2. Gene Ontology (GO) [4] has a unified representation of genes across all species. It consists of 130,094 axioms with 1,010 relations and 24,353 classes.
3. SNOMED CT [5] is a comprehensive ontology of clinical terms with 989,186 axioms, 307,712 classes and 60 relations.

4 PROPOSED APPROACH

In order to address the one-to-one relation restriction, we used a simple yet powerful technique that provides a foundation for further work in embeddings based description logic reasoning. We consider the relations to have a variance (uncertainty) leading to the translation having various possible regions in the vector space. This limits the capabilities of the model as most of the relations are many-to-many. We propose a modification to their approach, named $\text{EmEl(var)}$, to overcome the issue.

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Figure 1: Geometric representation of classes and relations. (a) shows the representation where $D \sqsubseteq C$ and thus the $n$-ball of $D$ lies inside $n$-ball of $C$. (b) shows class $C$ getting translated to $D$ using relation $R$ for a tuple $(C,R,D)$ in the ontology. (c) In case of $\text{EmEl(var)}$, the variance $\sigma$ lets the entity $C$ relate to multiple entities with the relation $R$. Any entity which falls within $\sigma$ distance of $C$-R is also related to $C$ through $R$. E and F are the boundary entities for $C$ and $R$.

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Baselines:

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(2) TransH [21]. In order to overcome the one-to-one problem as seen in TransE, it considers relations as hyperplanes and uses projection of entities on those hyperplanes to relate to other entities.

(3) DistMult [22]. A matrix factorization based model which has empirically performed well on compositional reasoning tasks.

(4) EmEl [11]. The embeddings take into consideration the structure of ontologies.

(5) EmEl++ [14]. An incremental work on top of EmEl with added properties like role inclusion and role chain.

5.1 Model Training
In order to train the embeddings, we use Pytorch [16] and its embedding layers. Pykeen framework [1] was used for implementing TransE, TransH, and DistMult embedding models. For EmEl embeddings, source code provided by the authors was used. In order to learn the embeddings for different models, we first normalize the ontologies, i.e., convert the axioms into one of the four normal forms discussed in Section 3. All individuals in the ontology are considered as nominal classes (containing one instance) and the embeddings learn to make their radii zero resulting in a point in the vector space. Next, we remove some of the subclass relation pairs for validation (20%) and testing (10%). Remaining 70% sub-class relation pairs are used for training the embedding functions.

5.2 Evaluation Metrics
Subsumption is one of the reasoning tasks and it checks whether the subclass relation exists between two classes. We chose subsumption to evaluate the effectiveness of the proposed embeddings rather than link prediction because this task makes use of the normalized axioms to infer the subclass relation. The task of subsumption is reduced as a distance-based operation in the embedding vector space. Given a test instance of the form \( C \subseteq D \), we use \( D \) as source class and rank all other classes in the given ontology in an increasing order of their distance from \( D \) in the vector space. Based on the rank at which \( C \) is present in the ranked list, we evaluate our model. We hypothesise that an embedding model that successfully captures the ontological information should be able to assign very close vector representations to the two classes in a subclass relation, hence, producing a lower rank for \( C \).

In order to evaluate the performance of different models, we use Hits at ranks 1, 10 and 100 which represent the fraction of the test cases where the given class \( C \) falls under top 1, 10 and 100 in rank list respectively. Median rank and 90\(^{th}\) percentile rank were also considered to compare the overall performance of the models. A median rank of \( m \) indicates that for 50% of test cases, the correct answer was found below rank \( m \). Similarly 90\(^{th}\) percentile rank indicates the rank below which the correct class was found for 90% of the test cases.

6 RESULTS
The evaluation results of the model on the subsumption task for all the three ontologies is given in Tables 1, 2 and 3 respectively. In all the three cases, EmEl(var) outperforms almost every other model across all the five metrics. The variants of EmEl perform better than other traditional KG Embeddings i.e. TransE, TransH and DistMult showing the importance of capturing underlying structures of the ontologies. EmEl++, in general, tends to perform slightly better than EmEl on various metrics as well. EmEl(var) improves the performance on the Galen ontology compared to the previous best performing models. A notable improvement is seen in the Top1 and Top100 values i.e. Top1 score increases from 0.02 in EmEl++ to 0.10 in EmEl(var) which is quite significant. Similarly, we see an increase of Top100 score from 0.19 in EmEl to 0.26 in EmEl(var).

Table 1: Performance of Different Methods for Galen

| Model  | Top1  | Top10 | Top100 | Median | 90th% Rank |
|--------|-------|-------|--------|--------|------------|
| TransE | 0.00  | 0.00  | 0.00   | 10748  | 21308      |
| TransH | 0.00  | 0.00  | 0.00   | 11721  | 21825      |
| DistMult | 0.00 | 0.00  | 0.00   | 12600  | 21823      |
| EmEl   | 0.01  | 0.11  | 0.19   | 6039   | 21221      |
| EmEl++ | 0.02  | 0.11  | 0.16   | 6623   | 20635      |
| EmEl(var) | 0.10 | 0.12  | 0.26   | 3540   | 19669      |

Table 2 shows a mixed result on the GO ontology. While EmEl(var) shows the best results for Top1, Top10 and Top100, it is comparable with EmEl++ in terms of the Median Rank and 90th Percentile Rank.

Table 2: Performance of Different Methods for GO

| Model  | Top1  | Top10 | Top100 | Median | 90th% Rank |
|--------|-------|-------|--------|--------|------------|
| TransE | 0.00  | 0.00  | 0.00   | 20079  | 40177      |
| TransH | 0.00  | 0.00  | 0.00   | 26280  | 41996      |
| DistMult | 0.00 | 0.00  | 0.00   | 22493  | 40425      |
| EmEl   | 0.01  | 0.08  | 0.15   | 9504   | 36447      |
| EmEl++ | 0.01  | 0.09  | 0.15   | 7232   | 33892      |
| EmEl(var) | 0.01 | 0.09  | 0.17   | 7542   | 34148      |

Table 3 contains results of our model on SNOMED CT, which is a large ontology. The Top1, Top10 and Top100 scores are significantly higher than any of the other models while the Median and 90th percentile ranks are less than half of the previous best performing models. This can be attributed to the fact that larger ontologies have larger relations that have many-to-many properties. EmEl(var) provides the model the freedom to incorporate those properties resulting in a substantially improved embedding.

Table 3: Performance of Different Methods for SNOMED CT

| Model  | Top1  | Top10 | Top100 | Median | 90th% Rank |
|--------|-------|-------|--------|--------|------------|
| TransE | 0.00  | 0.00  | 0.00   | 150876 | 274465     |
| TransH | 0.00  | 0.00  | 0.00   | 157186 | 278455     |
| DistMult | 0.00 | 0.00  | 0.00   | 151624 | 275982     |
| EmEl   | 0.00  | 0.03  | 0.08   | 80289  | 277874     |
| EmEl++ | 0.00  | 0.03  | 0.06   | 87413  | 261359     |
| EmEl(var) | 0.08 | 0.18  | 0.36   | 42759  | 134829     |
7 CONCLUSION

The existing Knowledge Graph and ontology embedding approaches assume that relations are one-to-one. This limits the possibility of using these embeddings for more expressive ontologies and for complex reasoning tasks. We have provided a simple yet effective method that overcomes this obstacle and helps embeddings to capture many-to-many relations. Through our evaluation, we have shown that our model outperforms the existing models in the subsumption task across three ontologies of varying sizes and characteristics. The technique that we described here, i.e., considering variance in relations, can be used in other knowledge graph embeddings such as TransE as well. The flexibility to model many-to-many relations also opens up the possibility of extending this work for more expressive description logics such as SROIQ.

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