Link Prediction in Knowledge Graphs: A Hierarchy-Constrained Approach

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Abstract—Link prediction over a knowledge graph aims to predict the missing head entities h or tail entities t and missing relations r for a triple (h, r, t). Recent years have witnessed great advance of knowledge graph embedding based link prediction methods, which represent entities and relations as elements of a continuous vector space. Most methods learn the embedding vectors by optimizing a margin-based loss function, where the margin is used to separate negative and positive triples in the loss function. The loss function utilizes the general structures of knowledge graphs, e.g., the vector of r is the translation of the vector of h and t, and the vector of t should be the nearest neighbor of the vector of $h + r$. However, there are many particular structures, and can be employed to promote the performance of link prediction. One typical structure in knowledge graphs is hierarchical structure, which existing methods have much unexplored. We argue that the hierarchical structures also contain rich inference patterns, and can further enhance the link prediction performance. In this paper, we propose a hierarchy-constrained link prediction method, called hTransM, on the basis of the translation-based knowledge graph embedding methods. It can adaptively determine the optimal margin by detecting the single-step and multi-step hierarchical structures. Moreover, we prove the effectiveness of hTransM theoretically, and experiments over three benchmark datasets and two sub-tasks of link prediction demonstrate the superiority of hTransM.

Index Terms—Link prediction, knowledge graph embedding, hierarchy

1 Introduction

A knowledge graph is a graph whose nodes represent entities and edges correspond to relations. As an effective organization of structural and non-structural information, large-scale knowledge graphs are constantly emerging, including Freebase [1], WordNet [2], OpenKN [3], Probase [4], etc. In the past decades, knowledge graphs have played a pivotal role in many areas such as semantic search, question answering systems and so on. However, all of them have a need to improve their coverage of facts, for which link prediction is an effective strategy and has been paid much attention [5], [6], [7], [8]. Link prediction is a task to predict missing edges under the supervision of given part of knowledge graphs. Since knowledge graphs are often represented as triples $\{(h, r, t)\}$, where h and t denote the head entities and the tail entities respectively, and r denotes the relation between them, link prediction over a knowledge graph aims to predict the missing triples i.e., to predict t (or h) given (h, r)(or (r, t)), or predict r given (h, t).

There is a quantity of techniques to tackle this problem, which mainly fall into two categories. The first category is rule-based and path-based methods, namely, the relations are predicted by explicitly learning the rules and the relation paths. One typical method is the First Order Inductive Learner, FOIL [9], [10], [11]. It conducts the predictive work mainly by learning first-order Horn clauses. And another typical method is Path-constrained Random walk Algorithm, PRA [12], [13]. It makes prediction from the aspect of structural information, i.e., the relation paths between entities. Compared to the rule-based predictive methods, the predictive performance using path-based methods has been greatly improved, which indicates that relation paths are of great use in predicting relations. Nevertheless, path-based methods fail to predict links well when faced with entities which have no relations with others before, and the performance of path-based methods plunges definitely for sparsely connected graph.

The second category is knowledge graph embedding based predictive methods, where the relations of entities are learned implicitly in the embedding vectors. Most methods embed a knowledge graph into a low-dimensional vector space according to a margin-based loss function, and then a score for each triple (h, r, t) is calculated based on score function $f_r(h, t)$. Finally, a list of candidate triples is returned in the decreasing order of their scores. The typical methods are translation-based methods, for example, TransE [14], which models relations r as translations from head entities h to tail entities t, i.e., $\mathbf{h} + \mathbf{r} \approx \mathbf{t}$, where $\mathbf{h}, \mathbf{r}, \mathbf{t} \in \mathbb{R}^d$ are the embedding vectors of h, r and t, respectively. Moreover, TransA [15] employs more structural information of knowledge graphs, i.e., the local distance of entities and the proximity of relations. The success of TransA indicates that the special structures in knowledge graphs can further enhance the link prediction performance. Furthermore, there are other methods that employ the particular structures to achieve better performance. For instance, inspired by PRA, PTransE [16] integrates the relation paths into the learning process, which improves the link prediction performance significantly.

However, there are many particular structures of knowledge graphs that are not taken full advantage of. One typical

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structure is the hierarchical structure, which is a structure where entities are organized in a tree, and their relations are hierarchical relations [17]. We argue that the hierarchical structures can further improve the link prediction performance, since there are also rich patterns contained similar to relation paths. In addition, hierarchical structures are extremely common in knowledge graphs due to the ubiquitousness of hierarchical relations. For instance, WN18, a subset of the knowledge graph WordNet, has about 50% hierarchical relations. Furthermore, hierarchical structures will lead to a special distribution of entities in the embedding space, which provides more constraints compared to non-hierarchical structures, so that the performance of link prediction will be promoted.

Motivated by this intuition, we propose a hierarchy-constrained link prediction method based on knowledge graph embedding, called hTransM. Specifically, we seek out a method to detect hierarchical structures and model them from two aspects, i.e., the single-step hierarchical structures and the multi-step hierarchical structures, and the optimal hierarchy-constrained margin is learned with respect to different hierarchical structures. As a result, the embedding vectors of the entities and relations of the knowledge graph can be trained under the supervision of hierarchical structures. Experiments are conducted over three benchmark datasets for two sub-tasks of link prediction, and the results demonstrate that the proposed method outperforms the state-of-the-art method. Specifically, the contributions of the paper are four-fold.

- We divide the hierarchical structures into two categories, i.e., single-step hierarchical structures and multi-step hierarchical structures. Besides, we provide one way to detect the hierarchical structures in knowledge graphs by employing the properties of hierarchical relations. Moreover, the influence of hierarchical structures on the performance of link prediction is analyzed in a intuitional way.
- We propose a hierarchy-constrained link prediction method based on knowledge graph embedding, called hTransM. According to whether the relations and relation paths that connect the entities are hierarchical or not, it finds the optimal loss function by adaptively determining the margins.
- We further prove the convergence of hTransM by demonstrating its uniform stability and provide the upper bound of the error of the proposed model. What's more, hTransM possesses the same model complexity (i.e., the number of parameters) as other simple methods such as TransE.
- Experiments over three benchmark datasets of two sub-tasks, i.e., entity prediction task and relation prediction task, suggest that the proposed method can achieve better prediction performance. Furthermore, the superiority of hierarchy-constrained margin is validated by experiments through studying the variation of the optimal margin value along with the optimization process, and compared with the methods which do not considering hierarchical information.

In the remainder of the paper, we present the related work on link prediction models in Section 2. Then we model the hierarchical structures in Section 3 and describe hTransM in detail in Section 4, the fast implementation in Section 5, and the convergence and model complexity in Section 6. After that, we detail an experimental study on three benchmark datasets by two sub-tasks of link prediction in Section 7, and draw the conclusion in Section 8.

2 Related Work

Link prediction in knowledge graphs, i.e., predicting links between entities, has received much attention in recent years. Since knowledge graphs are often represented as triples (h, r, t), the link prediction task can be formulated as predicting t given (h, r), or predicting h given (r, t), or predicting r given (h, t).

Existing link prediction methods mainly fall into two categories according to the ways in modeling the existing relation between entities. The first category is to explicitly model the existing relations, including rule-based and path-based methods. For example, FOIL [9], [10], [11] is a rule-based method by employing the first order inductive logic, and is followed by the models reducing manual work in defining rules, e.g., NELL [11], Sherlock-Holmes [18]. In the meanwhile, PRA [12], [13] is a typical path-based method, which models the existing relations by relation paths. The relation path is made up of the relations from the head entity to the tail entity, such as $p = \left(\cdot \xrightarrow{r_1} \cdot \xrightarrow{r_2} \cdot \xrightarrow{r_3} \dots \xrightarrow{r_l} \cdot\right)$, where l is the length of the relation path p. It regards the relation paths as training experts, and predicts the relations by ranking candidates in terms of the weighted score of these relation paths. PRA has achieved a great success in link prediction, which demonstrates the effectiveness of relation path information in link prediction task. Then, a bunch of methods [19], [20], [21] emerge to enrich the relation paths for better predictive performance. Besides, the relation paths already have been widely used in a quantity of applications, such as expert path finding [22], relation extraction based on KB structure [12] [23], etc. Although path-based methods greatly improve the link prediction performance, the performance of them is hampered for sparsely connected graph and they are not scalable quite well for large scale knowledge graphs.

The second category is to implicitly model the relations of entities, including knowledge graph embedding based predictive methods. According to the structures of the graph, these methods embed a knowledge graph into a low-dimensional latent space, and then a score function $f_r(h, t)$ for each triple (h, r, t) is learned. Finally, a list of candidate entities is returned in the decreasing order in term of their scores. In recent years, knowledge graph embedding based methods have received much attention, which mainly fall into two key branches, i.e., the translation-based methods and others. Translation-based models regard the relation of a triple as the translation from the head entity to the tail entity, including TransE [14], TransH [24], TransR [25], PTransE [16], TransA [15], etc. They usually define a margin-based loss function to separate the negative triples from positive triples in the embedding space.

TransE [14] is a pioneering work of Translation-based knowledge graph embedding methods. It models the embedding vector of relation $\mathbf{r}$ as translation from the head

entity embedding vector $\mathbf{h}$ to the tail entity embedding vector $\mathbf{t}$, i.e., $\mathbf{h}+\mathbf{r} \approx \mathbf{t}$, where $\mathbf{h}, \mathbf{r}, \mathbf{t} \in \mathbb{R}^d$ are the embedding vectors of h, r and t, and d is the dimension of embedding space. As a result, the score function for each triple (h, r, t) is $f_r(h, t) = ||\mathbf{h} + \mathbf{r} - \mathbf{t}||$, and the candidate triples are ranked in the decreasing order of their scores. TransE works well for 1-to-1 relations but has issues for N-to-1, 1-to-N and N-to-N relations. For instance, it can be derived that $h_0 = \ldots = h_i = \ldots = h_m$, for all (h_i, r, t) in the knowledge graph when r is a 1-to-N relation, where m is the number of these triples. This is obviously in conflict with the fact.

To address this issue, TransH [24] considers that the distance between h and t is distinct from different relations, and each relation represents a different hyperplane. Consequently, TransH formulates the relation as a projection transformation, namely, $f_r(h, t) = ||\mathbf{h}_\perp + \mathbf{r} - \mathbf{t}_\perp||$, where $\mathbf{h}_\perp = \mathbf{h} - \mathbf{w_r}^\top \mathbf{h} \mathbf{w_r}$ and $\mathbf{t}_\perp = \mathbf{t} - \mathbf{w_r}^\top \mathbf{t} \mathbf{w_r}$, with $\mathbf{w_r}$ as the normal vector of the hyperplane related to r. Furthermore, TransR [25] models the relation as a rotation transformation, namely, $f_r(h, t) = ||\mathbf{h_r} + \mathbf{r} - \mathbf{t_r}||$, where $\mathbf{h_r} = \mathbf{M_r h}$ and $\mathbf{t_r} = \mathbf{M_r t}$. In other words, it utilizes a projection matrix $M_r \in \mathbb{R}^{k \times d}$, where k is the dimension of the entity embedding vector space, and d is the dimension of the relation embedding vector space. Similar work also contains TransD [26] and TransM [27].

Besides translation-based embedding methods, there are also other models to learn the embedding vectors of the knowledge graphs. For example, energy-based methods aim to assign low energies to the triples and are optimized by neural networks. Unstructured model [28] is one of the typical energy-based models. It ignores the relation information and the score function is simplified to $f_r(h, t) = ||\mathbf{h}-\mathbf{t}||$. The Structured Embedding (SE) model [29] defines two matrix corresponding to the relations to transform the entities, and the score function is formulated as $f_r(h, t) = ||\mathbf{M_{h,r}} \mathbf{h} - \mathbf{M_{t,r}} \mathbf{t}||$. The Semantic Matching Energy (SME) model [30] formulates the score function by employing the correlations between entities and relations with two matrix operators, i.e., $f_r(h, t) = (\mathbf{M_1 h}+\mathbf{M_2 h}+\mathbf{b_1})^\top (\mathbf{M_1 h}+\mathbf{M_2 h}+\mathbf{b_2})$ using add operator, and $f_r(h, t) = (\mathbf{M_1 h} \otimes \mathbf{M_2 h} + \mathbf{b_1})^\top (\mathbf{M_1 h} \otimes \mathbf{M_2 h} + \mathbf{b_2})$ using Hadamard operator. The LFM model [31], [32] considers a quadratic form to model the second-order correlations between entity embedding vectors, and the score function is $f_r(h, t) = \mathbf{h}^\top \mathbf{M_r t}$.

Both TransE, TransH, TransR and other translation-based methods employ a fixed margin based loss function, and the value of the fixed margin is chosen during experiments. However, knowledge graphs exhibit different locality with regard to different types of entities and relations. Namely, when the entities and relations change, the optimal margin between the negative and positive triple scores should vary accordingly. Hence, TransA [15] determines the optimal margin adaptively. It employs the entity-specific margin, which is the local distance between negative and positive entities, and relation-specific margin, which is the proximity of relations. Since the predictive performance of TransA is fairly good, the effectiveness of structural information to promote the predictive performance has been verified. There are other methods improve the knowledge embedding performance by making use of the rich information of typical structures, such as PTransE [16]. It combines the loss generated by path $\sum_p \sum_{(h,r',t)} (||\mathbf{p} - \mathbf{r}|| - ||\mathbf{p} - \mathbf{r}'|| + M)$, where $\mathbf{p}$ is the embedding vector of the multi-step relation path p. TransA and PTransE significantly outperform the methods that do not utilize the special structure of knowledge graphs, which demonstrates the superiority of employing special structures in knowledge graphs.

As a result, we consider that one of the typical structures of knowledge graphs, i.e., hierarchical structure, contains rich inference information, and can be employed to promote the performance of link prediction. However, the existing knowledge graph embedding methods fail to utilize the rich information in hierarchical structures. More precisely, the hierarchical structure is a structure where entities are organized in a tree, and their relations are hierarchical relations [14]. Owing to its universality, the hierarchical structure has been explored a lot recently. Taxonomy Embedding [33] and Label Embedding Trees [34] are two approaches to leverage the taxonomy structure during embedding [35]. Taxonomy Embedding represents the class and entities into a latent semantic space that underlies the class hierarchy, and then the classification is done with simple nearest neighbor rule [33]. Label Embedding Trees approach aims to learn a tree-structure by optimizing the overall tree loss for multi-class classification [34].

Nevertheless, these methods mainly employ the hierarchical information by defining the entity similarity as the distance along the tree. Namely, they explore the hierarchical structures from the global aspect, which ignores the hierarchical information of a single-step, i.e., from local aspect. Actually, the hierarchical structures can be analyzed from two aspects, i.e., the single-step aspect and the multi-step aspect, both of which can provide rich information to promote the performance of link prediction. Consequently, we shall propose a hierarchy-constrained link prediction method based on knowledge graph embedding, to integrate both the single-step and multi-step hierarchical information into the predictive method.

3 Hierarchical Structure Formulation

In this section, we firstly describe hierarchical relations in knowledge graphs with an example for clear explanation, and seek out a way to distinguish them. Then, we formulate multi-step hierarchical relation path and hierarchical structures in detail.

3.1 Hierarchical Relation Formulation

Hierarchical structure is a structure where entities are organized into layers by one relation [36]. Different layers imply different vertical orders, and the meaning varies from relations. For instance, in the hierarchical structure organized by relation $child$, different layers indicate different generations, and the entities in the higher layers is senior to lower layers. Taking Fig.1 (a) as an example, $Barack\,Obama\,Sr.$, his child $Barack\,Obama$ and his two grandchildren $Sasha\,Obama$ and $Malia\,Obama$ compose a three-layer hierarchical structure by relation $child$, illustrated in Fig.1 (b). In this case, $Barack\,Obama\,Sr.$ is on the first layer, with $Barack\,Obama$ on the second layer, and $Sasha\,Obama$ and $Malia\,Obama$ on the third layer respectively. Actually, hierarchical structure is a directed network containing no cycles, which is

called a directed acyclic graph (DAG). It has been proved in [37], a DAG has a unique hierarchical structure, and each node can be labeled with a unique layer index, which is calculated using a recursive labeling algorithm.

Furthermore, the relations composing hierarchical structures are called hierarchical relations, e.g., the relation *child* in Fig.1. More formally,

Definition 1. **Hierarchical relation** is the relation that enables entities to be organized into layers.

Hierarchical relations between entities, such as *child* between *Barack Obama* and *Sasha Obama*, are relations between layers. That is to say, head entity and tail entity are on different layers. In addition, hierarchical relations have directions from the head entity to the tail entity, which means they are irreflexive.

On the contrary, **non-hierarchical relations** between entities, such as relation *colleague* between *Barack Obama* and *Hillary Clinton*, and relation *siblings* between *Sasha Obama* and *Malia Obama*, are relations that do not enforce the related entities to be on different layers, which means one can interchange the head entity with the tail entity of a triple, and the new triple obtained is still correct. Namely, non-hierarchical relations are reflexive.

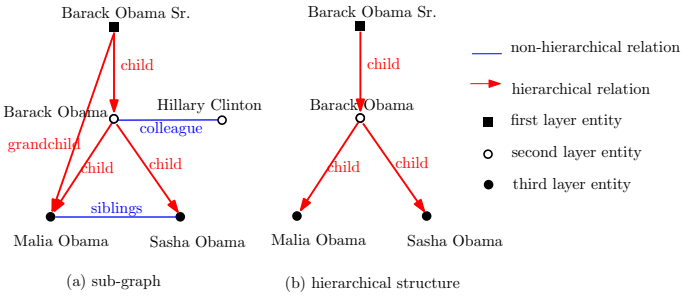

Fig. 1: Hierarchical and non-hierarchical relations in knowledge graphs, where (a) represents a sub-graph of knowledge graph, and (b) is the three-layered hierarchical structure extracted from it, which is composed by relation *child*.

One way to distinguish hierarchical relations in a knowledge graph is to study the reflexive properties and the mapping properties of relations. Following [14], mapping properties can be defined as follows: A given relation is *1-to-1* if a head can appear with at most one tail, *1-to-N* if a head can appear with many tails, and *1-to-1* and *N-to-N* analogously. As mentioned above, hierarchical relations should be irreflexive. In addition, the hierarchical relations are closely in accordance with mapping properties. That is to say, *1-to-N* (e.g., WordNet's *_hyponym*) or *N-to-1* (e.g., WordNet's *_hypernym*) relations are always hierarchical ones. On the contrary, *1-to-1* (e.g., *passport unique id*, *current spouse*) relations indicate unique relation for both head and tail entities, so that they can not be utilized to expand to multi-layered structures, and are not hierarchical relations. As for *N-to-N* relations, when the cardinalities of head and tail entities are almost the same (e.g., *siblings*, *colleagues*), the relations are non-hierarchical relations, but if there is a gap between the cardinalities, and the relations are not reflexive, (e.g. *parent_to_child*, *advisor_to_advisee*), the relations are always hierarchical relations. As a result, we detect the relations, which is irreflexive with unbalanced mapping properties, to be hierarchical relations. Notice that, utilizing reflexive properties and mapping properties of relations is just one way to discover hierarchical relations in the statistical sense, and may not hold for every single hierarchical relation.

Specifically, we detect the irreflexive relations by the proportion of irreflexive related triples to all related triples, where a triple is called irreflexive triple if it does not hold when interchanging its head and tail. Provided that the proportion is bigger than 50%, the relation is considered as irreflexive relation. For instance, in WN18 [14], a subset of WordNet, the proportion of irreflexive triples related to relation *_similar_to* is 7.5%, so that *_similar_to* is non-hierarchical relation. In addition, we follow the way in [14] to decide the mapping properties of relations in terms of the cardinalities of their head and tail arguments. Namely, if the average number of heads h (or tails t) for a relation is below 1.5, then the argument is labeled as 1, and N otherwise. For example, in WN18, relation *_also_see* has 1.65 heads per tail and 1.84 tail per head in average, so that it is labeled as *N-to-N*. Since the cardinalities of head and tail entities are quite similar, which is determined according to whether the difference of cardinalities is smaller than 1 in this paper, *_also_see* is not a hierarchical relation. On the contrary, *_hypernym* has an average of 3.67 heads per tail and of 1.02 tail per head, so it is labeled as *N-to-1*. Plus the proportion of irreflexive related triples is 100%, the relation *_hypernym* is detected as hierarchical relation consequently.

3.2 Hierarchical Relation Path Formulation

The **relation path** is made up of the relations from the head entity to the tail entity [12], e.g., the solid line in Fig.2 illustrates the relation paths extracted from Fig.1. Besides, it has been proved in [16] that, for a given entity pair (h, t), the relation paths p connecting (h, t) are consistent with the direct relation r between (h, t), since the relationships between (h, t) can be interpreted by both of them. In this case, we call the relation as **consistent relation** of the relation path. For instance, the paths (solid line in Fig.2) are highly correlated to the direct single-step relation (dotted line in Fig.2). Taking Fig.2 (a) as an example, the consistent relation of the relation path $\left(\xrightarrow{child} \cdot \xrightarrow{child}\right)$ is the relation *grandchild*.

Moreover, the relation path could be a hierarchical path or not. A relation path is a hierarchical relation path, if there is at least one hierarchical relation among the related relations. In this case, the head entities and tail entities are enabled to be on different layers. More formally,

Definition 2. **Hierarchical relation path** is a multi-step relation path $p = \left(\xrightarrow{r_1} \cdot \xrightarrow{r_2} \ldots \xrightarrow{r_l}\right)$, which satisfies

$$\exists i \in \{1, 2, \ldots, l\}, \quad r_i \in H_r,$$

where l is the length of the relation path, and H_r is the set of hierarchical relations in the knowledge graph.

Otherwise, the path is **non-hierarchical relation path**.

For instance, the relation path $\left(\xrightarrow{child} \cdot \xrightarrow{child}\right)$ in Fig.2 (a) is a hierarchical relation path, since it contains two hierarchical relations. Similarly, the other ten relation paths

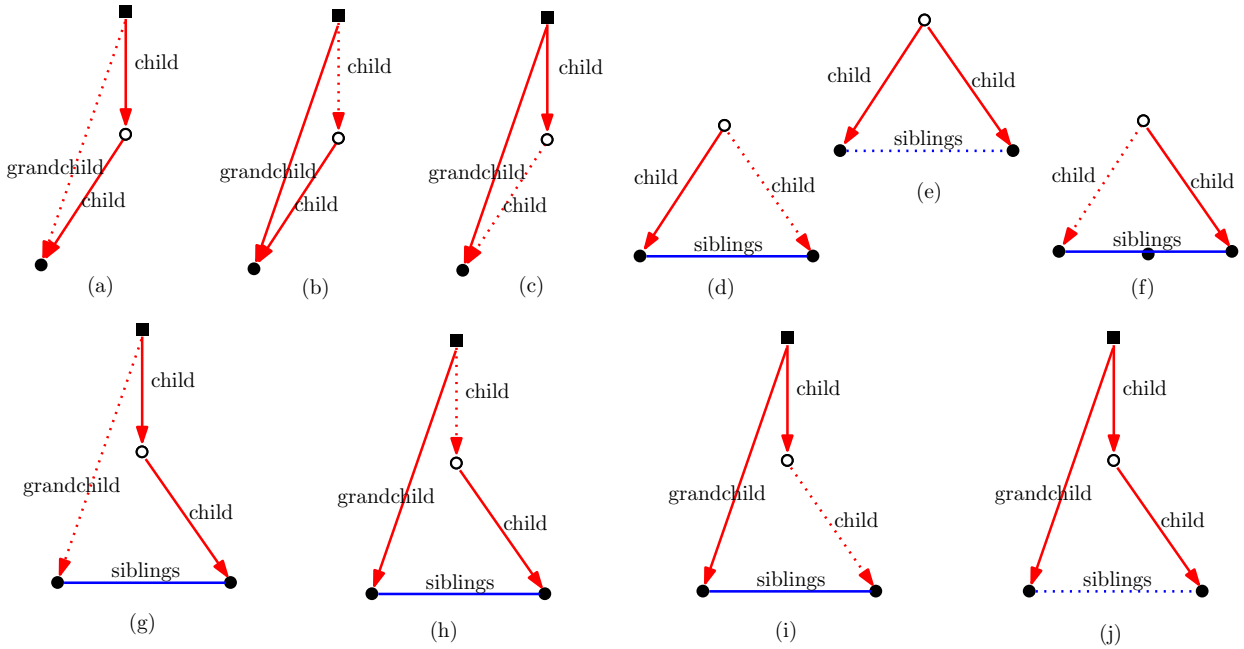

Fig. 2: Relation paths extracted from the knowledge graph in Fig.1, where the dotted edges represent the relation consistent with the path. For instance, the relation path $\left(\xrightarrow{child} \cdot \xrightarrow{child}\right)$ is highly correlated with the relation $grandchild$.

in Fig.2 (b) to Fig.2 (j) are all hierarchical paths, as they all possess at least one hierarchical relation.

Note that the relation paths in knowledge graphs consist of the reverse relations. For example, the triple ($Barack\,Obama$, $child$, $Malia\,Obama$) can be reversed to ($Malia\,Obama$, $child^{-1}$, $Barack\,Obama$), and $child^{-1}$ is the reverse relation of $parent$. Besides, the non-hierarchical relations are considered as existing in both directions, that is to say, ($Sasha\,Obama$, $siblings$, $Malia\,Obama$) and ($Malia\,Obama$, $siblings$, $Sasha\,Obama$) both hold, so the reverse relation of a non-hierarchical relation is itself.

3.3 Hierarchical Structure Formulation

Hierarchical structures are ubiquitous in knowledge graphs, since hierarchical relations widely exist. For example, FB15k and WN18, the subset from widely used knowledge graph WordNet and Freebase respectively, both have about 50% hierarchical relations at least. In addition, compared with the general relations, the entities connected by hierarchical relations will be distributed distinguishingly in the embedding space, since the hierarchical relations enforce the connected entities to be on different layers. Hence, it is intuitive that these constraints will contribute to the link prediction process. For Instance, knowing that $Sasha\,Obama$ is on the next layer of $Barack\,Obama$, helps to predict the relation $child$ between $Barack\,Obama$ and $Sasha\,Obama$.

Besides, the hierarchical structures imply two kinds of inference information that can be used to link prediction, i.e., the information of single-step hierarchical structures and the information of multi-step hierarchical structures. More precisely, we first define single-step structure and multi-step structure. The **single-step structure** is the structure where entities are connected by one-step relations. Namely, a single triple can be regarded as a single-step structure. For example, as shown in Fig.1, the relation $child$ and the connected entities, i.e., $Barack\,Obama$ and $Sasha\,Obama$, form a single-step structure.

Furthermore, single-step structures can be divided into hierarchical and general single-step structure, according to whether the relation is hierarchical or not. More formally,

Definition 3. **Hierarchical single-step structure** is a single-step structure, where the relation is hierarchical, and two entities are distributed on two different layers .

On the contrary, **general single-step structures** are composed by non-hierarchical relations. Taking Fig.1 as an example, the single-step structure composed by $Barack\,Obama$, $child$ and $Sasha\,Obama$ is a hierarchical single-step structure, since the relation $child$ is a hierarchical relation. Besides, the relation $siblings$ and the connected entities, i.e., $Sasha\,Obama$ and $Malia\,Obama$, also form a single-step structure, but it is a general single-step structure, since $siblings$ is a non-hierarchical relation.

Instead, the **multi-step structure** is the structure where entities are connected by a relation path, and the length of the relation path is larger than 1. For example, in Fig.2 (a), the relation path $\left(\xrightarrow{child} \cdot \xrightarrow{child}\right)$, its consistent relation $grandchild$ and three connected entities $Barack\,Obama\,Sr.$, $Barack\,Obama$ and $Malia\,Obama$ form a multi-step structure.

Moreover, multi-step structures can be classified into hierarchical and general multi-step structure, based on whether the relation paths and the consistent relations are all hierarchical or not. More formally,

Definition 4. **Hierarchical multi-step structure** is a multi-step structure, where the relation path and the consistent relation are both hierarchical, and the head and tail entities are distributed on two different layers.

Otherwise, the multi-step structure is **general multi-step structure**. For instance, the multi-step hierarchical structure in Fig.2 (a) is hierarchical, since the relation path is a hierarchical relation path, and the consistent relation is hierarchical, too. However, the multi-step structure in Fig.2 (e) is a general one. Although the relation path $p = \left(\xleftarrow{child} \cdot \xrightarrow{child}\right)$ is a hierarchical path, the consistent relation $siblings$ is non-hierarchical, and the head entity $Malia\,Obama$ and tail entity $Sasha\,Obama$ are on the same layer.

Compared to hierarchical single-step structure, the entities in hierarchical multis-step structure can be distributed on more than two layers. Actually, the hierarchical single-step structure aims to capture the **local** hierarchical structure of knowledge graphs, where entities are on neighbour layers. Namely, it focus on the inter-layer information. On the contrary, the hierarchical multi-step structure focuses on the **global** hierarchical structure, which looks upon the whole hierarchical structure, and considering the information across layers.

4 The Link Prediction Method

In this section, we propose hTransM to integrate hierarchical structures into the predictive work. First of all, we describe the key idea of hTransM to model the hierarchy-constrained margin. Then, the details of the hierarchy-constrained margin is illustrated from two aspects, namely, from the insights of single-step and multi-step hierarchical structures.

4.1 The Predictive Method hTransM

Since it has been verified in [15] that the appropriate value of M_{opt} will significantly improve the performance of link prediction, the idea of hTransM is to define a hierarchy-constrained margin M_{opt} by detecting the hierarchical and general structures, where M_{opt} is used to separate positive triples from negative triples. Specifically, the positive triples are the golden triples in the knowledge graph, denoted by $(h, r, t) \in \Delta$, and the negative triples are the corrupted triples that not exist in the knowledge graph, and are constructed by substituting one of the entities or the relations following [14], denoted by $(h', r', t') \in \Delta'$.

Then the embedding of entities and relations to a vector space $\mathbb{R}^d$ for each triple (h, r, t) is learned by minimizing a loss function concerning M_{opt},

$$L = \sum_{(h,r,t)\in\Delta} \sum_{(h',r',t')\in\Delta'} \max(0, f_r(h,t) + M_{opt} - f_r(h',t')) \tag{1}$$

where $\max(0, \cdot) = [\cdot]_+$ is the hinge loss. $f_r(h, t)$ is the score function for the triple (h, r, t). In this paper, the score function adopts the form defined in [14] without loss of generality,

$$f_r(h,t) = ||\mathbf{h} + \mathbf{r} - \mathbf{t}|| \tag{2}$$

where the boldface characters denote the embedding vectors of entities and relations in $\mathbb{R}^d$, and d is the dimension of the embedding space. For instance, $\mathbf{h}$ is the embedding vector of the entity h. And $||\cdot||$ is the L_1-norm or L_2-norm of the vector. In order to predict t given (h, r) or predict h given (r, t), candidate entities are ranked in terms of $f_r(h, t)$ and a list is returned in the decreasing order of $f_r(h, t)$.

Since hierarchical structures are fully composed of single-step hierarchical structures and multi-step hierarchical structures, the optimal hierarchy-constrained margin M_{opt} is modelled from two aspects, i.e., single-step aspect and multi-step aspect. Moreover, it is natural to linearly combine the two specific margins via parameters α, β to control the trade-off between them. Therefore, the optimal hierarchy-constrained margin satisfies

$$M_{opt} = \alpha M_{single} + \beta M_{multi} \tag{3}$$

where $0 \leq \alpha, \beta \leq 1$, M_{single} denotes the single-step specific margin and M_{multi} denotes the multi-step specific margin. For the sake of obtaining optimal hierarchy-constrained margin M_{opt}, it is sufficient to find the optimal single-step specific margin M_{single} and the optimal multi-step specific margin M_{multi}, so we will elaborate the setting of two margins respectively in the following.

4.2 Single-step Specific Margin

For a given triple (h, r, t), the single-step specific margin is generated according to the corresponding single-step specific structure. Firstly, let us denote some notations. For a given entity h and its related relation r, the set of positive entities, denoted by P_r, contains entities that have relation with h of type r. And the set of negative entities, denoted by N_r, contains entities that have relations with h of other relation r'.

Provided that the single-step structure is a general one, it has been verified in [38] that, for a given head entity h and relation r, the optimal performance is achieved when the embedding vectors bring positive tail entities P_r close to each other, and move negative tail entities N_r away with a margin. Hence, the positive entities should be closer to h than the negative ones. Namely, the distance from positive entities $t \in P_r$ to h, i.e. $||\mathbf{h} - \mathbf{t}||$, should be shorter than the distance from negative entities $t' \in N_r$ to h, i.e., $||\mathbf{h} - \mathbf{t}'||$. Furthermore, when the difference between $||\mathbf{h} - \mathbf{t}'||$ and $||\mathbf{h} - \mathbf{t}||$ obtains minimum, the difference between them is exactly the margin. As a result, $\min(||\mathbf{h} - \mathbf{t}'|| - ||\mathbf{h} - \mathbf{t}||), t \in P_r, t' \in N_r$ is introduced to model the difference between the distance from P_r to h and the distance from N_r to h. Specifically, the minimum difference obtains when it takes the nearest negative entity (red rectangle in Fig.3) and the farthest positive entity (red circle in Fig.3). From geometry aspect, the margin of general single-step structure is the distance between two concentric spheres, illustrated in Fig.3. This definition is kind of similar to the margin defined in Support Vector Machine [39], [40], where the margin of two classes is equal to the minimum absolute distance of any two different-class instances to the classification hyperplane. Notice that the above analysis applies to both the head entity h and the tail entity t, here we simply take head entity h as an example in the rest of the paper.

Provided that the single-step structure is a hierarchical one, it has been mentioned in [14] that the siblings are close to each other considering the natural representation of trees. Namely, the positive entities of h should lie close to each other in a small area, since they are siblings with h

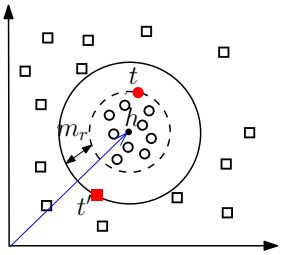

Fig. 3: The illustration of the general single-step specific margin, where circles stand for positive entities and rectangles represent negative ones in the embedding space $\mathbb{R}^d$.

as the common father. In other words, the positive entities can be enclosed in a circular sector (shaded area in Fig.4). It means that, when separating the negative examples from the positive ones, the negative entities near the circular sector (red rectangle in Fig.4) plays more important role, rather than the negative entities with small distance to h but actually away from the circular sector (black rectangle in Fig.4). As a result, the nearest negative entity that used to determine margin should not only have small distance with h, but also close to the circular sector. As a result, we introduce an angle θ to model this hierarchy-constraint, where θ is the angle between the vector $\mathbf{h}-\mathbf{t_i'}$ and the vector $\mathbf{h}-\mathbf{t_i}$. Consequently, we applied a regularization parameter with respect to θ to force the nearest negative entity that determining the margin close to the circular sector.

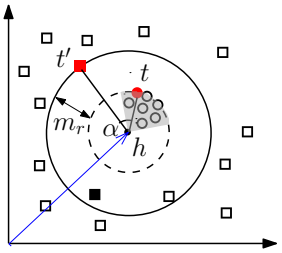

Fig. 4: The illustration of the hierarchical single-step specific margin, where circles stand for positive entities and rectangles represent negative ones in the embedding space $\mathbb{R}^d$.

Formally, for a given triple (h, r, t), M_{single} is defined as the average of m_r for different relations r related to h (or t), where m_r is the margin between P_r and N_r for the given r and h (or t). More formally, taking h as an example,

$$M_{single} = \frac{\sum_{r \in R_h} m_r}{|R_h|}, \tag{4}$$

where R_h is the set of all relations related to h and $|R_h|$ is the cardinality of R_h.

Moreover, m_r is defined according to whether r is hierarchical or not. Specifically, let H_r be the set of hierarchical relations in a knowledge graph. Then for all $t \in P_r$ and $t' \in N_r$, we define

$$m_r = \begin{cases} \min_{t,t'} \sigma(||\mathbf{h}-\mathbf{t}'|| - ||\mathbf{h}-\mathbf{t}||), & r \notin H_r \\ \min_{t,t'} \sigma(||\mathbf{h}-\mathbf{t}'|| - ||\mathbf{h}-\mathbf{t}||) + \lambda_{hr}\phi(\theta), & r \in H_r \end{cases} \tag{5}$$

where

$$\sigma(x) = \begin{cases} x & \text{when } x \geq 0; \\ -x & \text{otherwise.} \end{cases} \tag{6}$$

returns the absolute value of x. Here, θ is the angle between the two vectors $\mathbf{h}-\mathbf{t}$ and $\mathbf{h}-\mathbf{t}'$ in the vector space $\mathbb{R}^d$. $\phi(\theta) = 1 - \cos\theta$ is penalty function which is monotonically increasing with respect to θ, so that the penalty increases when θ becomes larger, and approximates zero when θ is close to zero. λ_{hr} is a regularization parameter to leverage the penalty, which satisfies $0 \leq \lambda_{hr} \leq 1$. More formally,

$$\lambda_{hr} = \exp\left[-\frac{1}{|E_{h,r}|}\right], \tag{7}$$

where $E_{h,r}$ is the set of tail entities of the given h and r, and $|E_{h,r}|$ is the cardinality of $E_{h,r}$. Notice that λ_{hr} is monotonically increasing with respect to $|E_{h,r}|$, which means the larger $|E_{h,r}|$ is, the more the siblings t has, leading to increasing penalty. In particular, when $N_r = \emptyset$, we set $m_r = 0$, which is reasonable since all positive entities are within the internal sphere. And when $P_r = \emptyset$, we set $m_r = \min_{t'} ||\mathbf{h}-\mathbf{t}'||$ to move the negative entities away.

Actually, the margin with penalty of θ can be regarded as soft margin, which is similar to the margin defined in Support Vector Machine, to avoid overfitting. Namely, the negative examples with small distance but large θ is not fairly close to the positive entities, and the errors caused by them are allowed while fitting the model.

4.3 Multi-step Specific Margin

To define the multi-step specific margin for a given triple (h, r, t), the relation paths connecting h and t are extracted, and are used to generate corresponding multi-step structures with r as consistent relation. Above all, let us give some notations. For a given multi-step relation path p, the set of positive relations, denoted by P_p, contains the consistent relations r. If p connects h and t, the positive relations r connect them as well, which form the golden triples (h, r, t) in the knowledge graph. On the contrary, the set of negative relations, denoted by N_p, contains the relations r' that are not consistent with p. If p connects h and t, the negative relations r' is obtained by replacing the relation r of golden triples (h, r, t), such that the corrupted triple (h, r', t) does not exist in the knowledge graph.

Provided that the multi-step structure is a general one, there are three conditions, according to the hierarchical properties of the relation paths and the consistent relations. 1) Firstly, supposing that the path p is non-hierarchical relation path and the consistent relation r is non-hierarchical relation, they should be close to each other in the embedding space [16], i.e., $\mathbf{p} \approx \mathbf{r}$, since they connect the same entities, and both can be regarded as translation from the same head to same tail entities. As a result, for a given p, the positive relations $r \in P_p$ should be closer to p than the negative relations $r' \in N_p$. Similar to general single-step specific margin, we introduce $\min(||\mathbf{r}'-\mathbf{p}|| - ||\mathbf{r}-\mathbf{p}||), r \in P_p, r' \in N_p$ to model the margin between positive and negative relations. Hence, the margin is determined by the nearest negative relation (red square in Fig.5) and furtherest positive relation (red circle in Fig.5). From geometry aspect, the positive relations (circles in Fig.5) are constrained within the internal

sphere, along with the negative relations (squares in Fig.5) outside the external sphere. Hence, as illustrated in Fig.5, the general multi-step specific margin should be the distance between two concentric spheres in the embedding space. 2) Secondly, supposing that the path is hierarchical but the relation is not, owing to the existence of reverse relation, it is possible that the two entities connected by the path are on the same layer, e.g., the multi-step structure in Fig.2 (e) (j). As a result, there is little difference whether the relation path is hierarchical or not. In this case, the margin is the same as above. 3) Thirdly, supposing that the relation is hierarchical but the path is not, the relation forces head and tail entities to be on different layers, which is conflict with the hierarchical property of path. Hence, this case can be regarded as no positive relations. Namely, the margin calculation is the same as above, except clearing the positive relations before calculation.

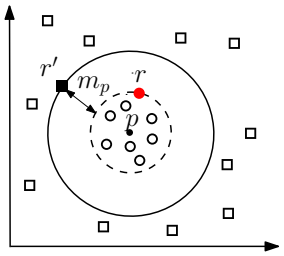

Fig. 5: The illustration of m_p, where circles stand for positive relations and rectangles represent negative relations in the embedding space $\mathbb{R}^d$.

Provided that the multi-step structure is a hierarchical one, the path and the consistent relation are both hierarchical. Since the hierarchical relations force the head and tail entities to be on different layers, the consistent relation paths should be hierarchical, which enables the head and tail entities to be on different layers. That is to say, the hierarchical relation paths are highly correlated to hierarchical relations, and are indispensable for the existence of hierarchical relations. Hence, the hierarchical relation paths should be paid more attention than non-hierarchical ones when detecting the optimal margin. To this end, we introduce μ_p, which is the proportion of hierarchical relations to all relations contained in p. More formally,

$$\mu_p = \frac{|\{r : r \in p \wedge r \in H_r\}|}{|\{r : r \in p\}|}, \tag{8}$$

where $|\cdot|$ is the cardinality of the set. For instance, the relation path in Fig.2 (a), $p = \left(\xrightarrow{child} \cdot \xrightarrow{child}\right)$, is hierarchical relation path, and the consistent relation $grandchild$ is hierarchical as well. As there are two hierarchical relations in this path, $\mu_p = \frac{2}{2} = 1$. Similarly, Fig.2 (b) (c) (d) (f) (g) (h) (i) are hierarchical relation paths, and have hierarchical consistent relations, μ_p equals 1, 1, 0.5, 0.5, 0.67, 0.67, 0.67 respectively.

Formally, for a given triple (h, r, t), the multi-step specific margin M_{multi} is the weighted average of m_p for different paths p consistent to r, where m_p denote the margin between P_p and N_p. More formally,

$$M_{multi} = \begin{cases} \dfrac{\sum_{p \in Path_{h,t}} [(1+\mu_p) R(p|h,t) m_p]}{\sum_{p \in Path_{h,t}} [(1+\mu_p) R(p|h,t)]}, \\ \qquad\qquad p \in H_p \wedge r \in H_r \\ \dfrac{\sum_{p \in Path_{h,t}} [R(p|h,t) m_p]}{\sum_{p \in Path_{h,t}} R(p|h,t)}, \\ \qquad\qquad p \notin H_p \vee r \notin H_r \end{cases} \tag{9}$$

where $Path_{h,t}$ is the set of relation paths connecting h and t, and H_p denotes the set of hierarchical relation paths in the knowledge graph, with H_r the set of hierarchical relations in knowledge graphs.

Specifically, m_p is defined as follows. Given r and p, for all $r \in P_p$ and $r' \in N_p$,

$$m_p = \min_{r,r'} \sigma(||\mathbf{r}' - \mathbf{p}|| - ||\mathbf{r} - \mathbf{p}||), \tag{10}$$

where

$$\sigma(x) = \begin{cases} x & \text{when } x \geq 0; \\ -x & \text{otherwise.} \end{cases} \tag{11}$$

returns the absolute value of x. And $\mathbf{r}, \mathbf{r}', \mathbf{p} \in \mathbb{R}^d$ denote the embedding vectors of r, r', p respectively. Note that the embedding vector of p can be composed of the embedding vectors of entities following [16]. In this paper, the add operator is adopted as it achieved the best performance in [16]. Namely, $\mathbf{p} = \mathbf{h} + \mathbf{r_1} + \mathbf{r_2} + \cdots + \mathbf{t}$. In particular, similar to single-step specific margin, we set $m_p = 0$ if $N_p = \emptyset$, and set $m_p = \min_{r'} ||\mathbf{r}' - \mathbf{p}||$ when $P_p = \emptyset$.

Besides, $R(p|h,t)$ represents the reliability of a relation path p for the given entities h and t, and it is determined by the resource amount that eventually flows to the tail entity t from the head entity h along the path p by the path-constraint resource allocation algorithm following [16]. More precisely, for a relation path $p = \left(e_0 \xrightarrow{r_1} e_1 \xrightarrow{r_2} e_2 \xrightarrow{r_3} \ldots \xrightarrow{r_l} e_l\right)$, the resource flowing to a entity m, which is connected by the path p, is defined as follows,

$$R_p(m) = \sum_{n \in S_{i-1}(\cdot,m)} \frac{1}{|S_i(n,\cdot)|} R_p(n), \tag{12}$$

where $S_{i-1}(\cdot, m)$ is the direct predecessors of m along relation r_i, and $S_i(n, \cdot)$ represents the direct successors of n along relation r_i. Note that for the path between h and t, $e_0 = h$ and $e_l = t$. Besides, the initial resource of h is set to 1 in general, i.e., $R_p(h) = 1$. In the meanwhile, the reliability of a relation path p is measured by resource amount flows to t, i.e., $R(p|h,t) = R_p(t)$.

Furthermore, another application of the reliability score is to filter the unreliable paths, since candidate paths can be numerous, and the unreliable path may even drag down the predictive performance. Similar path selection techniques can be found in [41] [42] [43].

5 The Implemention of hTransM

The learning process of hTransM is carried out by stochastic gradient descent (SGD) in minibatch mode, and the initialization of all embedding vectors of entities and relations follows the random procedure in [44], [14]. Comparing to the

TransE, there is an additional novel hierarchy-constrained margin computation procedure, which is conducted once every iteration for one triple.

The detailed training procedure is described in Algorithm 1. Firstly, all the relation paths with length less than l are discovered by traversing the knowledge graph employing Breadth-First-Search (BFS), and a reliable score is assigned for each relation path according to Eq. (12). Note that the reverse relations should be constructed following Section 3.2. After that, the reliable paths, whose reliable score is larger than threshold, is selected to form the set of reliable paths $Path_{h,t}$ for each for each $(h,r,t) \in S$. Secondly, the initialization procedure is conducted for all entities and relations. Thirdly, the optimization using SGD is conducted.

Let M_s denote the set of optimal single-step specific margin for all triples, and M_m be the set of optimal multi-step specific margin for all triples. At each main iteration of the algorithm, M_s and M_m will be cleared at first, and a novel set of triples and corresponding corrupted ones are sampled. In the meanwhile, for a given triple, the margin computation procedure will firstly check whether the margin of the training triple has been calculated in the current iteration, then the optimal margin calcluation is only carried out for the triples whose margin are not known. This strategy reduces the repeated calculation and leads to high efficiency. Then the embedding vectors are updated based on the optimal margin. At last, the algorithm will be stopped on the basis of the performance on a validation set.

Note that this procedure could be applied to any margin based knowledge graph embedding method, since it is a general framework to choose margin adaptively for the sake of better performance.

Algorithm 1 Training hTransM

Require:
Training set $S = \{(h,r,t)\}$, entities and relations set E and R, embedding dimension d, path length l, parameters $\alpha, \beta, \lambda, \mu$;
Ensure:
Embeddings of entities and relations;
Find and select reliable relation path set $Path_{h,t}$ for each $(h,r,t) \in S$
Initialize $r \in R$ and $e \in E$ by uniform distribution
loop
  $\mathbf{e} \leftarrow \frac{\mathbf{e}}{||\mathbf{e}||}$ for each entity $e \in E$
  $S_{batch} \leftarrow sample(S, b)$ //sample a minibatch of size b
  $T_{batch} \leftarrow \emptyset$
  $M_s \leftarrow \emptyset$
  $M_m \leftarrow \emptyset$
  for all $(h,r,t) \in S_{batch}$ **do**
    $(h',r,t') \leftarrow sample(S'_{(h,r,t)})$ //sample a corrupted triple
    $T_{batch} \leftarrow T_{batch} \cup \{(h,r,t),(h',r,t')\}$
    if $M_{single}(h,r,t) \notin M_s$ **then**
      Calculating $M_{single}(h,r,t)$ by Eq. (4)
      $M_s \leftarrow M_s \cup \{M_{single}\}$
    end if
    if $M_{multi}(h,r,t) \notin M_m$ **then**
      Calculating $M_{multi}(h,r,t)$ by Eq. (9)
      $M_m \leftarrow M_m \cup \{M_{multi}(h,r,t)\}$
    end if
  end for
  for all $\{(h,r,t),(h',r,t')\} \in T_{batch}$ **do**
    Calculating M_{opt} by Eq. (3)
    Calculating $\nabla[f_r(h,t) + M_{opt} - f_r(h',t')]$
  end for
  Update embeddings of entities and relations w.r.t. $\sum_{\{(h,r,t),(h',r,t')\} \in T_{batch}} \nabla[f_r(h,t) + M_{opt} - f_r(h',t')]$
end loop

6 Analysis of hTransM

In this section, the convergence of hTransM is proved by demonstrating its uniform distribution, and model complexity is analyzed by employing parameter size.

6.1 The Convergence of hTransM

The convergence of hTransM is analyzed by studying the uniform stability instead of directly proving the uniform convergence following [15], since it has been proved that uniform stability is a sufficient condition for learnability of learning problem [45].

To show the effectiveness of a learning algorithm $\mathcal{A}$, the generalization error, i.e., true risk, is used generally, which can not be calculate directly and often approximated by the empirical risk. Let the training data set is denoted by $S = \{(h_1,r_1,t_1),\ldots,(h_i,r_i,t_i),\ldots,(h_n,r_n,t_n)\}$, where n is the size of the training set. $\mathcal{R}_{emp}(\mathcal{A},S)$ stands for the empirical risk, and $\mathcal{R}(\mathcal{A},S)$ for the true risk. Provided that the training data S is drawn independent and identically distributed (i.e., i.i.d.) from an unknown distribution $\mathcal{D}$, hTransM is said to be convergent if the empirical risk $\mathcal{R}_{emp}(\mathcal{A},S)$ converges to the true risk $\mathcal{R}(\mathcal{A},S)$, where

$$\mathcal{R}(\mathcal{A},S) = \mathbb{E}_z[\mathcal{L}(\mathcal{A},z)], \tag{13}$$

$$\mathcal{R}_{emp}(\mathcal{A},S) = \frac{1}{n}\sum_{k=1}^{n}\mathcal{L}(\mathcal{A},z_k), \tag{14}$$

where $z = (h,r,t)$ is a triple sampled according to $\mathcal{D}$, $z_k = (h_k,r_k,t_k)$ is the k-th element of S, $k \in \{1,2,\cdots,n\}$, and $\mathbb{E}_z[\cdot]$ denotes the expectation. To this end, we define the Uniform-Replace-One stability motivated by [45].

Definition 5. The learning algorithm $\mathcal{A}$ has Uniform-Replace-One stability γ with respect to the loss function $\mathcal{L}$ for $i \in \{1,2,\ldots,n\}$, the following inequality holds

$$\|\mathcal{L}(\mathcal{A}_S,\cdot) - \mathcal{L}(\mathcal{A}_{S^i},\cdot)\|_\infty \leq \gamma. \tag{15}$$

where

$$S^i = \{S \backslash (h_i,r_i,t_i) \cup (h'_i,r_i,t'_i)\}, \tag{16}$$

Here, $\mathcal{A}_S$ means that the learning algorithm $\mathcal{A}$ is trained on the data set S, and $\|\cdot\|_\infty$ is the maximum norm. h'_i and t'_i are the corrupted entities. The loss function $\mathcal{L}$ of hTransM takes the form

$$\mathcal{L}(\mathcal{A}_S,z) = f_r(h,t) + M_{opt} - f_r(h',t'), \tag{17}$$

from which we have the following lemma.

Lemma 6. The Uniform-Replace-One stability γ of hTransM with respect to the given loss function $\mathcal{L}(\mathcal{A}_S,z)$ is equal

to $2\hat{f}_r + 2\hat{R}$, where $\hat{f}_r = \max_{h,t} f_r(h,t)$ is the maximum over the triples $(h,r,t) \in S$, and $\hat{R} = 2R_{ent} + 2R_{rel} + 2$ with R_{ent} be the radius of the smallest sphere containing the learning entities, and R_{rel} be the radius of the smallest sphere containing the learning relations .

Proof: By Eq.(15) and Eq.(17) we deduce that

$$\begin{aligned}
&\|\mathcal{L}(\mathcal{A}_S,\cdot) - \mathcal{L}(\mathcal{A}_{S^i},\cdot)\|_\infty = \max_{z_i} |\mathcal{L}(\mathcal{A}_S, z_i) - \mathcal{L}(\mathcal{A}_{S^i}, z_i)| \\
&= |f_r(h,t) + M_{opt} - f_r(h',t') - (f_r(h,t) + M'_{opt} - f_r(h'',t''))| \\
&\le |f_r(h'',t'') - f_r(h',t')| + |M_{opt} - M'_{opt}| \\
&\le |f_r(h'',t'')| + |f_r(h',t')| + |M_{opt}| + |M'_{opt}| \\
&\le 2\max_{h,t} f_r(h,t) + |M_{opt}| + |M'_{opt}|.
\end{aligned}$$

where h', t' are the corrupted entities for $\mathcal{L}(\mathcal{A}_S,\cdot)$ and h'', t'' for $\mathcal{L}(\mathcal{A}_{S^i}, z_i)$. By Eq.(5) and definition of R_{ent}, we can deduce that

$$m_r \le \sigma(||\mathbf{h} - \mathbf{t}'|| - ||\mathbf{h} - \mathbf{t}||) + \lambda_{hr}\phi(\theta) \le 2R_{ent} + 2,$$

since $0 \le \lambda_{hr} \le 1$ and $0 \le \phi(\theta) \le 2$. Namely, $m_r \le \hat{R}$. Similarly, by Eq.(10) and definition of R_{rel}, it can be deduced that

$$m_p \le \sigma(||\mathbf{r}' - \mathbf{p}|| - ||\mathbf{r} - \mathbf{p}||) \le 2R_{rel}.$$

This leads to

$$M_{opt} \le \alpha 2R_{ent} + \beta 2R_{rel} + 2 \le \alpha 2R_{ent} + \beta 2R_{rel} + 2,$$

i.e., $M_{opt} \le \hat{R}$ by Eq.(3). Setting $\hat{f}_r = \max_{h,t} f_r(h,t)$ completes the proof. □

Then, the difference between two risks can be derived.

Theorem 7. For the embedding method $\mathcal{A}$ with Uniform-Replace-One stability γ with respect to the given loss function $\mathcal{L}$, we have the following inequality with probability at least $1-\delta$,

$$\mathcal{R}(\mathcal{A},S) \le \mathcal{R}_{emp}(\mathcal{A},S) + \sqrt{\frac{(\hat{R}+\hat{f}_r)^2}{2n\delta} + \frac{6\hat{f}_r(\hat{R}+\hat{f}_r)}{\delta}}, \tag{18}$$

Before proving Theorem 7, we first present the following Lemma verified in [45].

Lemma 8. For any algorithm $\mathcal{A}$ and loss function $\mathcal{L}(\mathcal{A}_S, z)$ such that $0 \le \mathcal{L}(\mathcal{A}_S, z) \le \hat{L}$, set $z_i = (h_i, r_i, t_i) \in S$, we have for any different $i, j \in \{1, 2, \ldots, n\}$ that

$$\begin{aligned}
&\mathbb{E}_S\left[\left(\mathcal{R}(\mathcal{A},S) - \mathcal{R}_{emp}(\mathcal{A},S)\right)^2\right] \\
&\le \frac{\hat{L}^2}{2n} + 3\hat{L}\mathbb{E}_{S\cup z'_i}[|\mathcal{L}(\mathcal{A}_S, z_i) - \mathcal{L}(\mathcal{A}_{S^i}, z_i)|]
\end{aligned}$$

Proof of Theorem 7: First, from Eq.(17), we deduce that

$$\mathcal{L}(\mathcal{A}_S, z) \le M_{opt} + f_r(h,t) \le \hat{R} + \hat{f}_r.$$

Then from Definition 5, we find that

$$\mathbb{E}_{S\cup z'_i}[|\mathcal{L}(\mathcal{A}_S, z_i) - \mathcal{L}(\mathcal{A}_{S^i}, z_i)|] \le \gamma.$$

Hence, by Lemma 8 and Lemma 6, we obtain that

$$\mathbb{E}_S\left[\left(\mathcal{R}(\mathcal{A},S) - \mathcal{R}_{emp}(\mathcal{A},S)\right)^2\right] \le \frac{(\hat{R}+\hat{f}_r)^2}{2n} + 6(\hat{R}+\hat{f}_r)\hat{f}_r$$

By Chebyshev's inequality, it can be derived that

$$\begin{aligned}
&Prob((\mathcal{R}(\mathcal{A},S) - \mathcal{R}_{emp}(\mathcal{A},S)) \ge \epsilon) \\
&\le \frac{\mathbb{E}_S\left[\left(\mathcal{R}(\mathcal{A},S) - \mathcal{R}_{emp}(\mathcal{A},S)\right)^2\right]}{\epsilon^2} \\
&\le \left(\frac{(\hat{R}+\hat{f}_r)^2}{2n} + 6(\hat{R}+\hat{f}_r)\hat{f}_r\right)\cdot\frac{1}{\epsilon^2}.
\end{aligned}$$

Let the right hand side of the above inequality be δ, then we have with probability at least $1-\delta$ that

$$\mathcal{R}(\mathcal{A},S) \le \mathcal{R}_{emp}(\mathcal{A},S) + \sqrt{\frac{(\hat{R}+\hat{f}_r)^2}{2n\delta} + \frac{6\hat{f}_r(\hat{R}+\hat{f}_r)}{\delta}}.$$

This completes the proof. □

6.2 Model Complexity of hTransM

The model complexity of hTransM is studied from the aspect of model parameters, which has been widely used to evaluate the complexity of knowledge graph embedding methods [14], [46], [24]. The number of parameters of hTransM is the same as other simple embedding methods, e.g., TransE [14], HOLE [46], since the main parameters of hTransM is the embedding vectors for each entity and each relation. As a result, the number of model parameters of hTransM is $\mathcal{O}(dn_e + dn_r)$, where n_e denotes the number of entities in a knowledge graph, and n_r represents the number of relations in a knowledge graph. d stands for the embedding dimension.

The comparison and the values for a typical knowledge graph FB15k (in millions) are illustrated in detail in TABLE1, where the embedding dimension is set to 100 for all methods. Besides, the statistics of the FB15k is shown in TABLE2.

TABLE 1: Numbers of parameters and their values for FB15k (in millions) with the embeddings dimension d = 100, where n_e and n_r are the number of entities and relations .

Method	Model complexity	on FB15k
RESCAL	$\mathcal{O}(dn_e + n_r d^2)$	14.9M
TransE	$\mathcal{O}(dn_e + dn_r)$	1.6M
TransH	$\mathcal{O}(dn_e + 2dn_r)$	1.8 M
TransR	$\mathcal{O}(dn_e + dn_r + n_r d^2)$	15.1M
PTransE	$\mathcal{O}(dn_e + dn_r)$	1.6M
HOLE	$\mathcal{O}(dn_e + dn_r)$	1.6M
TransA	$\mathcal{O}(dn_e + dn_r)$	1.6M
hTransM	$\mathcal{O}(dn_e + dn_r)$	1.6M

7 Experiments

The experiments are carried out on three public knowledge graphs, WN18 introduced in [14], FB15k introduced in [14] and FAMILY introduced in [47]. WN18 and FB15k are subsets of the widely used knowledge graph WordNet and Freebase respectively. FAMILY is an artificial hierarchical knowledge graph expressing family relationships among the members of 5 families along 6 generations, where entities are organized in a layered tree. The statistics of the datasets are listed in TABLE2.

Moreover, to detect the hierarchical relations, firstly the relations are classified into *1-to-1*, *1-to-N*, *N-to-1*, *N-to-N* and the proportion of the four classes are 25.5%, 17.4%, 30.9%,

26.2% on WN18, 31.3%, 27.2%, 21.5%, 20.0% on FB15k, and 0.3%, 32.0%, 19.0%, 48.7% on FAMILY. Note that FAMILY is constructed to capture the hierarchical structures in the knowledge graph, thus the *1-to-1* is little. Secondly, we find the irreflexive relations by calculating the proportion of irreflexive related triples, and the set of hierarchical relations is the union of irreflexive relations and unbalanced *1-to-N*, *N-to-1* and *N-to-N* relations. After that, the proportion of hierarchical relations is 77.8% on WN18, 53.9% on FB15k, and 42.9% on FAMILY. Experiments are conducted on two subtasks of link prediction, i.e., Entity Prediction and Relation Prediction.

TABLE 2: The datasets.

Datasets	# Relation	# Entitiy	#Train	#Valid	#Test
WN18	18	40,943	141,442	5,000	5,000
FB15k	1,345	14,951	483,142	50,000	59,071
FAMILY	7	721	8,461	2,820	2,821

7.1 Entity Prediction

This task aims to predict the missing entities h or t for a triple (h, r, t). Namely, it predicts t given $(h, r, \cdot)$ or predict h given $(\cdot, r, t)$. Similar to the setting in [14], [16], [15], for entity prediction, a list of candidate entities is returned in terms of the score function Eq. (2) of hTransM, and Mean Rank is adopted as the evaluation measure, which is the average rank of correct entities in original triples . It is clear that a good predictor has low mean rank. This is called "Raw" setting. We also filter out the corrupted triples which are correct ones for evaluation following [14], which called "Filter" setting. Namely, If a corrupted triple exists in the knowledge graph, it is also acceptable to rank it ahead the original triples. To eliminate this case, the "Filter" setting is more preferred [16].

The baseline methods include classical embedding methods, such as Unstructured [28], RESCAL [48], SE [29], SME [30], LFM [31], [32], TransE [14], TransH [24], TransR [25], PTransE [16], TransA [15] as shown in TABLE3. Since the datasets WN18 and FB15k are also used by the baseline methods, the experimental results are compared with those reported in their papers. Note that the results of FAMILY of those baselines are obtained by employing the publicly available code, as no results are reported in the papers.

For the parameter tuning process, we determine their values in the same way as the existing methods. The learning rate η during the SGD process is selected among $\{0.1, 0.01, 0.001\}$, the embedding dimension d in $\{50, 100, 200, 300, 400, \cdots, 800\}$, the batch size B among $\{120, 480, 1440, 4800\}$, and parameters α and β in $[0, 1]$. All parameters are determined on the validation set. Specifically, for hTransM, the optimal settings are: $\eta = 0.001$, $d = 200$, $B = 1440$, $\alpha = 0.9$, $\beta = 0.1$ on WN18, and taking L_1 as dissimilarity. $\eta = 0.001$, $d = 700$, $B = 1440$, $\alpha = 0.1$, $\beta = 0.3$ on FB15k, as well as taking L_1 as dissimilarity. $\eta = 0.001$, $d = 50$, $B = 120$, $\alpha = 0.7$, $\beta = 0.1$ on FAMILY, as well as taking L_1 as dissimilarity.

It can tell from TABLE3 that on all the datasets, i.e., WN18, FB15k and FAMILY, hTransM obtains the lowest mean rank. Moreover, hTransM decreases the mean rank by $20\% \sim 30\%$ on WN18 compared to TransA, which performs best among all the baselines. Besides, the decrease of Mean Rank on WN18 is larger than FB15k and FAMILY. It is unsurprising since the proportion of hierarchical relations are far bigger than FB15k and FAMILY, which proves the superiority of employing hierarchical structures to promote the performance of entity prediction.

TABLE 3: Evaluation results on entity prediction.

Data sets	WN18		FB15k		FAMILY	
Metric	Mean Rank		Mean Rank		Mean Rank	
	Raw	Filter	Raw	Filter	Raw	Filter
Unstructured	315	304	1,074	979	374	357
RESCAL	1,180	1,163	828	683	-	-
SE	1,011	985	273	162	362	351
SME(linear)	545	533	274	154	26	9
SME(bilinear)	526	509	284	158	29	12
LFM	469	456	283	164	-	-
TransE	263	251	243	125	29	8
TransH(bern)	401	388	212	87	-	-
TransH(unif)	318	303	211	84	-	-
TransR(bern)	238	225	198	77	26	7
TransR(unif)	232	219	226	78	25	7
PTransE(2-step)	245	237	200	54	24	7
PTransE(3-step)	245	238	207	58	24	7
TransA	165	153	164	58	23	6
hTransM	131	119	160	47	19	5

For further analysis, we calculated the predictive results according to different relation types, i.e., hierarchical and non-hierarchical relations, respectively. Since TransA performs best in TABLE3, the detailed results on three datasets are just compared with TransA, as listed in TABLE4. Note that the filter Mean Rank is adopted to do further analyzing, as the "Filter" setting is more comport with the fact. Besides, "hie" represents hierarchical relations, and "non-hie" represents non-hierarchical relations.

TABLE 4: Filtered Mean Rank of different relation types.

Measure Metric		WN18		FB15k		FAMILY	
		hie	non-hie	hie	non-hie	hie	non-hie
All	TransA	168	445	103	135	5.7	177
	hTransM	136	415	80	111	3.9	122
Head	TransA	133	478	113	129	4.4	177
	hTransM	123	419	87	108	3.1	122
Tail	TransA	203	411	94	141	6.8	177
	hTransM	151	410	73	113	4.8	122

It can be seen from TABLE4 that the decreases of mean rank on different types of relations are different. hTransM achieves larger decrease on hierarchical relations than non-hierarchical ones, which makes sense since when given a hierarchical relation, it is more possible that the layer of predicted entity is different from the layer of the given entity. Besides, the decrement of Mean Rank is different on predicting head and tail entities, i.e., the decrement is larger on the worse side of TransA, especially on WN18. For instance, TransA perform worse on predicting tail for hierarchical relations, as well as predicting head for non-hierarchical relations, while hTransM decrease far more on these two sides than the other sides. It is caused by the unbalanced mapping properties of relations, and the worse predicting side of TransA is the side with large cardinality, which demonstrates that hTransM can handle relations with unbalanced mapping properties.

7.2 Relation Prediction

This task aims to predict the missing relation r for two given entities $(h, \cdot, t)$. Similar to the setting in [16], given entity pair (h, t), relation prediction returns a list of candidate relations, and Mean Rank is adopted as the evaluation measure, which is the average rank of correct relations in original triple. The corrupted triples which are correct ones are filtered out for evaluation following [14] similar to entity prediction sub-task.

The baseline methods for comparison include TransE [14], TransA [15], TransR [25] and PTransE [16], which it can be seen that the performance of these methods are fairly better than the others in entity prediction sub-task, thus are adopted as baselines in this sub-task. WN18 and FB15k are adopted as datasets. Besides, the number of relations on FAMILY is so little that Mean Rank is very low for all methods, thus it is unsufficient to verify the relation prediction performance, and is not adopted in this experiment. Since the results of entity prediction of these baselines are not reported in the paper, we employ the publicly available code of them to obtain the results.

For the parameter tuning process, we determine their values in the same way as the existing methods. Similar to entity prediction sub-task, the learning rate η during the SGD process is selected among $\{0.1, 0.01, 0.001\}$, the embedding dimension d in $\{50, 100, 200, 300, 400, \cdots, 800\}$, the batch size B among $\{120, 480, 1440, 4800\}$, and the parameter α, β in $[0, 1]$. All parameters are determined on the validation set. The optimal settings for hTransM are: $\eta = 0.001$, $d = 150$, $B = 1440$, $\alpha = 0.9$, $\beta = 0.1$ on WN18, and taking L_1 as dissimilarity. $\eta = 0.001$, $d = 700$, $B = 1440$ and the smoothing factors are set to $\alpha = 0$, $\beta = 0.3$ on FB15k, as well as taking L_1 as dissimilarity.

TABLE 5: Evaluation results on relation prediction.

Data sets	WN18		FB15k	
Metric	Mean Rank		Mean Rank	
	Raw	Filter	Raw	Filter
TransE	2.6	2.6	2.8	2.5
TransR(bern)	2.5	2.5	38	37
TransR(unif)	2.6	2.6	29	29
TransA	1.6	1.6	1.5	1.1
PTransE(2-step)	2.4	2.4	1.7	1.2
PTransE(3-step)	3.4	3.4	1.8	1.4
hTransM	1.5	1.5	1.5	1.0

The results in TABLE5 indicate that hTransM outperforms all the baselines on both WN18 and FB15k. Similar to the performance on WN18 is better than FB15k, due to the larger proportion of hierarchical relations in WN18. It makes sense that the hierarchical structures, which hTransM employs, can bring more room for the improvement of relation prediction, since the entities on different layers are supposed to connect by hierarchical relations. Furthermore, the result that TransA performs better that other baselines, also demonstrates the superiority of detecting the optimal margin adaptively.

7.3 Discussion about Hierarchy-contrained Margin

To better understand how the margin affects the predictive method, the value of the optimal hierarchy-constrained margin is plotted along with the iterations of SGD. Since TransA is another method adaptively determine the optimal margin for each triples, in order to compare the optimal margin generated by both methods, the experiment is conducted by hTransM and TransA. The dataset adopts WN18, FB15k and FAMILY without loss of generality. To avoid randomness, the margin is the average margin of all triples in a single iteration.

The process of margin variation is shown in Fig.6, where the x-axis represents the number of SGD iterations in the training process, and the y-axis represents the value of the optimal margin. Note that since a negative sampling procedure is carried out when generating the optimal margin, there exists randomness in Fig.6. As the number of triples in FAMILY is very small, the randomness of negative sampling on FAMILY is much more obvious than the other two datasets. There are three observations from Fig.6 as follows.

- Firstly, it is verified that the optimal margin becomes larger with the iterations of SGD increasing, which implies that adaptively choosing margin is consistent with the intrinsic characteristic of the margin-based knowledge graph embedding methods. It makes sense that the positive and negative examples have growing distance along with the optimization processing. Consequently, determining the optimal margin adaptively is of great assistance to the performance of link prediction.
- Secondly, it can tell that the hierarchy-constrained margin of hTransM is larger than general margin of TransA, and increase more rapidly as well. It validates that hierarchy-constrained margin can be regarded as soft margin, and it is effective by integrating the hierarchical information into the predictive method.
- Thirdly, the value and the convergence of optimal margin vary from different datasets. The earlier the convergence is, the faster the value of margin increases, and there will be a small decrease if the convergence comes very early, such as WN18.

8 Conclusion

In this paper, we study the link prediction problem on knowledge graphs. To make full use of the hierarchical structures of knowledge graphs, this paper proposes a hierarchy-constrained link prediction method based on knowledge graph embedding, called hTransM. It determines the margin adaptively to achieve optimal predictive performance. The margin is modelled by discovering hierarchical structures automatically, and dividing them into the single-step hierarchical structures and multi-step hierarchical structures, which contributes to the optimal single-step margin and optimal multi-step margin. Moreover, the paper demonstrates the effectiveness of the proposed method theoretically by studying the convergence and model complexity. Furthermore, experiments conducted on three datasets with two sub-tasks, i.e., entity prediction and relation prediction, validate the superiority of hTransM on link prediction task in knowledge graphs, and the validity of the hierarchy-constrained margin has been proved by experiments. In addition, the methods could be scaled to other margin-based translation embedding methods, such

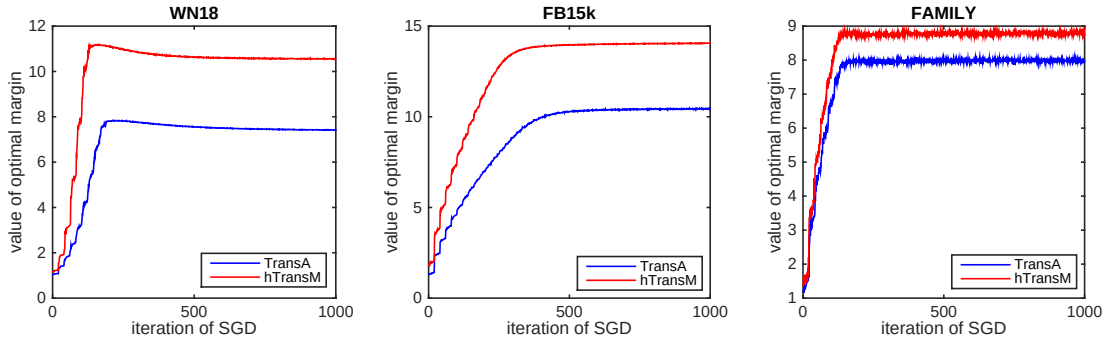

Fig. 6: The impact of the number of SGD iterations on the single-step margin of one entity on FAMILY, where x-axis stands for the number of sampling the triple in the training process, as well as the y-axis for the value of the margin.

as TransH, TransR, etc., on account of the effectiveness of the optimal margin.

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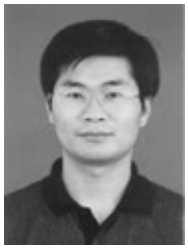

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