Modeling Relation Path for Knowledge Graph via Dynamic Projection

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***Abstract*— The application of representation learning in knowledge graphs has been a hot topic in recent years. Using representation learning methods, the semantic information contained in knowledge graphs can be embedded into low-dimensional dense vector spaces to achieve the purpose of efficiently processing knowledge graphs. A large number of research results have proved the advantage of the representation learning model represented by the translation model in processing knowledge graph related tasks. However, most translation models focus on the direct relation between entities and ignore the multi-hop relation between entities in the knowledge graph. In this paper, the relation path between entities in the knowledge graph is modeled. Considering the diversity of entities and relations in the knowledge graph, we embed entities and relations into different semantic spaces, and project the embedding results to the same space dynamically, while maintaining the consistency of the relation path between entities. We use benchmark datasets to evaluate the performance of the proposed model on the task of knowledge completion. The experiment shows that the model proposed in this paper is of great significance to solve the problem of knowledge completion in the knowledge graph.**

***Index Terms*—knowledge graph, dynamic projection, relation path**

I. Introduction

The knowledge base is a systematic and structured embodiment of human knowledge and is an important basic technology for intelligent information service applications such as intelligent search, intelligent question answering, and intelligent recommendation. Major search engines and organizations have also established multiple large knowledge bases to serve their products. Common English knowledge bases include Wikipedia, Probase, language knowledge base WordNet [1], and world knowledge base Freebase [2]. Chinese knowledge bases include Baidu Encyclopedia, Sogou Encyclopedia. Knowledge graph is a way to sort out and store information. It was first proposed by Google in 2012. Its essence is a knowledge base of the semantic network. Knowledge graphs have strong semantic expression capabilities, flexible modeling, a human-recognizable, machine-friendly way of expressing knowledge. It's the mainstream form of knowledge base. However, in the form of network representation, people need to design a special graph algorithm to store and utilize the knowledge base, which has the disadvantage of being time-consuming and laborious and is plagued by the problem of data sparseness.

Faced with this problem, representation learning in the field of deep learning has attracted people's attention. Representation learning is to represent the semantic information of the studied object as a low-dimensional dense real-valued vector, and in this space, the two objects with higher semantic similarity are closer. In the field of knowledge graphs, researchers can use representation learning to embed the entities in the knowledge graph and the relations between entities into a low-dimensional dense space, while retaining the semantic relations in the knowledge graph as much as possible. This method can improve the utilization efficiency of graph data and alleviate the problem of data sparseness.

By using representational learning to model the knowledge graph, people can easily achieve the task of completing the knowledge graph and discover the implicit relations among entities to expand the knowledge graph. However, most of the existing models cannot effectively use the multi-hop relation in the knowledge graph, and to some extent, the information hidden in the data is ignored.

This paper explores the application of representation learning in knowledge graphs, focusing on the effects of translation models on knowledge graph completion, and proposes a new model of the relation path between entities in the knowledge graph. The main contributions include:

1) This paper studied and summarized common translation models, and compared the advantages and disadvantages of different models.
2) We combine the construction ideas of PTransE [3] and TransD [4] to model the relation paths in the knowledge graph and proposed a new translation model, PTransD.
3) By evaluating the result of the knowledge completion task with the PTransD model in the benchmark data set, we verify the effectiveness of the model.

The rest of the paper is organized as follows. Related work is presented in Section II. In Section III, we detail our approach. The experiments and results of the proposed model will be introduced in Section IV. The conclusion we draw and feature work is presented in Section V.

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II. Related Work

In the field of knowledge graphs, translation models using representation learning are mainly used to solve the problems of knowledge representation and reasoning. The translation model mainly learns the structural features of the knowledge graph, namely (head entities, relations, and tail entities) triples, embeds entities and relations into low-dimensional dense spaces, and uses vectors to represent entities and relations. Since the TransE model [5] was proposed in 2013, a series of models have been produced to improve and supplement the TransE model, such as TransH [6], TransR [7], TransD [4], PTransE [3] and so on. This section mainly introduces these models.

A. TransE

In the TransE model, triples in the knowledge graph are denoted by (h, r, t). Correspondingly, their column vector are denoted by $\mathbf{h}, \mathbf{r}$ and $\mathbf{t}$. The mean idea of TransE is that the relation $\mathbf{r}$ is considered as the translation from $\mathbf{h}$ to $\mathbf{t}$. Therefore, the goal of the TransE model is to make $\mathbf{t} - \mathbf{h}$ equal to $\mathbf{r}$ as much as possible. The score function is defined as

$$f_r(\mathbf{h}, \mathbf{t}) = \|\mathbf{h} + \mathbf{r} - \mathbf{t}\|_{L_1/L_2} \tag{1}$$

where L_1/L_2 represents the 1-norm or 2-norm.

However, the TransE model embeds entities and relations into the same space, and for the same relation, different head and tail vectors may be close in distance. Therefore, the TransE model encounters difficulties when dealing with complex relation modeling.

B. TransH

The TransH model [6] overcomes the shortcomings of the TransE model's insufficient processing capacity for complex relations and makes the same entity vector have different representations under different relations.

The TransH model assumes that there is a corresponding hyperplane for each relation r, and the relation r falls on the hyperplane. Each entity can be projected onto the hyperplane where the relation r is located. Then the translation process similar to the TransE model will be performed on this hyperplane.

Let $\mathbf{h}_\perp$ and $\mathbf{t}_\perp$ represent the projected vector of head entity and tail entity respectively. The score function of the TransH model is defined as

$$f_r(\mathbf{h}, \mathbf{t}) = \|\mathbf{h}_\perp + \mathbf{r} - \mathbf{t}_\perp\|_{L_1/L_2} \tag{2}$$

Although the TransH model makes the same entity have different representations through projection under different relations, the model assumes that entities and relations are in the same semantic space, which limits its representation ability to a certain extent.

C. TransR

Both the TransE and TransH models assume that entities and relations are vectors in the same semantic space so that similar entities will be in similar positions in space. The TransR model believes that each entity can have many aspects, and different relations focus on different aspects of the entity, so different relations should have different semantic spaces. For each relation r, a transition matrix $\mathbf{M}_r$ is set. Entity vectors will be projected to the relation space with these matrices. The score function of TransR is

$$f_r(\mathbf{h}, \mathbf{t}) = \|\mathbf{M}_r\mathbf{h} + \mathbf{r} - \mathbf{M}_r\mathbf{t}\|_{L_1/L_2} \tag{3}$$

The TransR model separates the original single semantic space into entity space and relation space, which improves the model's representation ability. However, the transition matrix is only relevant to the relation, and the matrix multiplication increases the complexity of operations.

D. TransD

By using the dynamic mapping matrix, TransD [4] overcomes the above shortcomings of the TransR model to some extent. It uses different mapping methods to project entity vectors to the relation space. Besides the embedding vector, TransD constructs a projection vector for each entity or relation to build the dynamic mapping matrix. When the dimension of entity space and relation space is set to be the same, the score function of TransD can be simplified as

$$f_r(\mathbf{h}, \mathbf{t}) = \left\|\mathbf{h} + \mathbf{r} + (\mathbf{h}_p^T\mathbf{h} - \mathbf{t}_p^T\mathbf{t})\mathbf{r}_p - \mathbf{t}\right\|_{L_1/L_2} \tag{4}$$

where subscript p marks the projection vectors.

E. PTransE

The PTransE model [3] believes that in addition to direct relations in knowledge graphs, indirect relations reached between entities through other entities should also be of great significance for completing completion tasks in the knowledge graph. Therefore, PTransE models the relation paths between entities and gives quantitative calculations for the reliability of different relation paths. Using the relation paths, the PTransE model uses ideas similar to the TransE model to perform semantic relations in the knowledge graph Learn and complete the embedding of the knowledge graph.

PTransE solves two important challenges of using relational paths: i) the reliability calculation of relational paths, and ii) the semantic representation of relational paths. The PTransE model proposes a PCRA (Path-constraint Resource Allocation) algorithm based on the resource allocation algorithm in the network [8] and calculates the reliability of the relational path. The basic idea of the algorithm is that on a subgraph with entity h as the starting point and entity t as the ending point, it is assumed that a certain amount of resources flow out from h through the relation path, and the number of resources that can finally reach t reflects the reliability of the relation path.

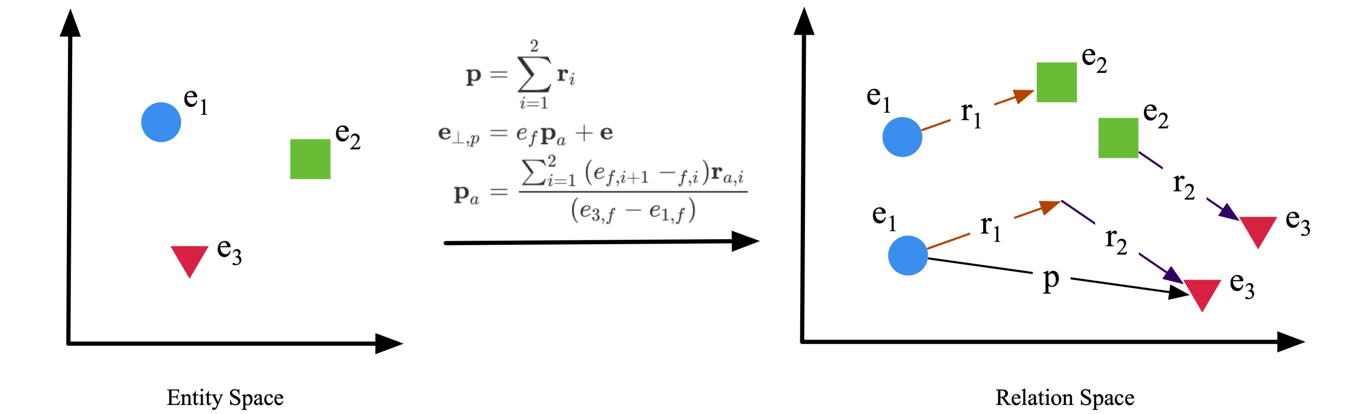

Fig. 1. Simple illustration of PTransD. Each shape represents an entity. There exists a relation path p between entity e_1 and entity e_3, which is denoted as $p = (r_1, r_2)$. With the auxiliary vector $\mathbf{p}_a$ of p, entities corresponding to p are projected from entity space to relation space. Notice that projections of e_2 changes according to its corresponding relation r_1 and r_2.

III. Our Method

In the TransD model, the entities and relations of the knowledge graph are embedded in different semantic spaces, and the entity vector is projected into the relation space by using a projection matrix. In the relation space, the equation $\mathbf{h} + \mathbf{r} = \mathbf{t}$ holds approximately. Since the projection matrices corresponding to the head entity and the tail entity are related to the entity itself and the relation, and the mathematical operation of the projection operation can eliminate the matrix multiplication operation, the TransD model becomes a more advanced model in the translation model.

The TransD model only considers the direct relation between entities when using knowledge graph data. The PTransE model is the first to propose the use of multi-step relations between entities in the knowledge graph. By setting the credibility of the relation path between entities, the PTransE model has also shown its importance in many translation models.

We draw on the advantages of the above two models and propose the PTransD model.

A. Model Description

For knowledge graph G, the semantic space to which the entity is mapped is $\mathbb{E}^k$, the semantic space to which the relation is mapped is $\mathbb{R}^k$, where k represents the spatial dimension. There are entity semantic vectors $\mathbf{h}, \mathbf{t} \in \mathbb{R}^k$ and relation vectors $\mathbf{r} \in \mathbb{R}^k$. To project the entity vector to the semantic space where the relation vector is located, and make use of the information on the structure of the knowledge graph, similar to the TransD model, PTransD model set auxiliary vectors $\mathbf{h}_a, \mathbf{t}_a$, and $\mathbf{r}_a$ for each semantic vector to construct a mapping matrix.

First we consider the case where the length of the relation path is 1, that is, the relation path between the head vector $\mathbf{h}$ and the tail vector $\mathbf{t}$ is the direct relation r between them. We will deduce this to a more general case.

Let $x_f = \mathbf{x}_a^T \mathbf{x}$ be the feature value corresponding to each entity. The PTransD model constructs a mapping matrix under the relation r for each head entity and tail entity by

$$\begin{aligned} \mathbf{M}_{rh} &= \mathbf{r}_a \mathbf{h}_a^T + \mathbf{I} \\ \mathbf{M}_{rt} &= \mathbf{r}_a \mathbf{t}_a^T + \mathbf{I} \end{aligned} \tag{5}$$

where $\mathbf{I}$ represents the identity matrix. Then using a mapping matrix, the projection of the head and tail entities in the semantic space where the relation r is located is:

$$\begin{aligned} \mathbf{h}_{\perp,r} &= \mathbf{M}_{rh}\mathbf{h} = h_f \mathbf{r}_a + \mathbf{h} \\ \mathbf{t}_{\perp,r} &= \mathbf{M}_{rt}\mathbf{t} = h_f \mathbf{r}_a + \mathbf{t} \end{aligned} \tag{6}$$

The goal of PTransD is to make the equation $\mathbf{h}_{\perp,r} + \mathbf{r} = \mathbf{t}_{\perp,r}$ approximately true. When the Equation (5) and Equation (6) holds, we have that

$$\mathbf{r} = (t_f - h_f)\mathbf{r}_a + \mathbf{t} - \mathbf{h} \tag{7}$$

More generally, for the triplets in knowledge graph $(h, r_0, x_1), (x_1, r_1, x_2), \ldots, (x_l, r_l, t)$, the relation path from h to t is marked as $p_r = (r_0, r_1, \ldots, r_l)$. Let $x_0 = h, x_{l+1} = t$, the entity path from h to t is marked as $p_e = (x_0, x_1, \ldots, x_{l+1}$. The vector of relation path is $\mathbf{p} = \mathbf{r}_0 \circ \mathbf{r}_1 \circ \cdots \circ \mathbf{r}_l$, where $\circ$ is a binary operator. In the PTransD model, we use the plus sign of vector as the binary operator. Under these conditions, the relation path vector is

$$\mathbf{p} = \sum_{i=1}^{l} \mathbf{r}_i \tag{8}$$

With Equation (7) and Equation (8), we can infer that

$$\begin{aligned} \mathbf{p} &= \sum_{i=1}^{l} \mathbf{r}_i = \sum_{i=1}^{l} [(x_{f,i+1} - x_{f,i})\mathbf{r}_{a,i} + \mathbf{x}_{i+1} - \mathbf{x}_i] \\ &= \sum_{i=1}^{l} (x_{f,i+1} - x_{f,i})\mathbf{r}_{a,i} + \mathbf{t} - \mathbf{h} \\ &= (t_f - h_f)\mathbf{p}_a + \mathbf{t} - \mathbf{h} \end{aligned} \tag{9}$$

That is

$$\mathbf{p}_a = \frac{1}{(t_f - h_f)} \sum_{i=1}^{l} (x_{f,i+1} - x_{f,i}) \mathbf{r}_{a,i} \tag{10}$$

The general goal of PTransD is to make the equation $\mathbf{h}_{\perp,p} + \mathbf{p} = \mathbf{t}_{\perp,p}$ hold among different entities.

An important idea in the PTransE model is that different relation paths have different degrees of reliability. The PTransD model follows this idea. For a triplet (h, p, t) given by the relation path $p = (r_1, r_2, \ldots, r_l)$, the possible path from h to t is $S_0 \xrightarrow{r_1} S_1 \xrightarrow{r_2} \ldots \xrightarrow{r_l} S_l$, where $S_0 = \{h\}$ and $t \in S_l$. For arbitrary entity $m \in S_i$, the set of the direct predecessor entities in S_{i-1} linked by r_i is noted as $S_{i-1}(\cdot, m)$. For arbitrary entity $n \in S_{i-1}$, the set of the direct successor entities in S_i linked by r_i is noted as $S_i(n, \cdot)$. The reliability degree is calculated with

$$R_p(m) = \sum_{n \in S_{i-1}(\cdot, m)} \frac{1}{|S_i(n, \cdot)|} R_p(n) \tag{11}$$

Let $R_p(h) = 1$, then $R_p(t)$ will shows the reliability of path p, noted as $R(p|h,t)$. An example for calculating the reliability of the relation path is shown in Fig 2. Then, the score function of PTransD is defined as

$$f_p(\mathbf{h}, \mathbf{t}) = \|\mathbf{h}_{\perp,p} + \mathbf{p} - \mathbf{h}_{\perp,t}\|_{L_1/L_2} \tag{12}$$

The set of golden path triplets is noted as Δ_p, which means that for any triplet $(h, p, t) \in \Delta_p$, there exists a relation path p from h to t, and the set of corrupt path triplets is $\Delta'_p = \{(h, p, t')|(h, p, t') \notin \Delta_p\} \cup \{(h', p, t)|(h', p, t) \notin \Delta_p\}$. We define the loss function of PTransD as

$$\mathcal{L} = \sum_{\mathbf{h},\mathbf{p},\mathbf{t} \in \Delta_p} \sum_{\mathbf{h}',\mathbf{p}',\mathbf{t}' \in \Delta'_p} C_p [f_p(\mathbf{h}, \mathbf{t}) - f_{p'}(\mathbf{h}', \mathbf{t}') + \gamma]_+ \tag{13}$$

where C_p is the confidence of relation path p. Let $P(h, t)$ be the set of all relation path from h to t, C_p is calculated by

$$C_p = \frac{R(p|h,t)}{\sum_{p \in P(h,t)} R(p|h,t)} \tag{14}$$

B. Relations among PTransD, TransD, and PTransE

It can be seen from the construction process of the PTransD model that when the length of the relation path in the PTransD model is limited to 1 and the reliability of the relation path is ignored, the PTransD model degenerates into a special form of TransD. At this time, the dimensions of the entity vector space and the relation vector space are the same in the TransD model.

Compared with the PTransE model, the PTransD model believes that the direct relation between entities is also an embodiment of the relation path. When calculating the model loss, the direct relation and the relation path can be treated the same, thereby simplifying the form of the loss function. The PTransD model retains the calculation ideas for path reliability proposed in the PTransE model and optimizes it. Besides, the PTransE model embeds entities and relations into the same space, while the PTransD model refers to the idea of the TransD model to embed entities and relations into different spaces, and complete the projection of the entity vector into the relation space dynamically. Thereby, the semantic structure of the knowledge graph can be modeled more clearly.

C. Knowledge Graph Completion

Although a common knowledge graph may have millions of entities and hundreds of millions of relations, these graphs may still be relatively sparse. Knowledge graph completion is to discover new information through the existing knowledge graph. According to the different objects in the triad of knowledge graph to be completed, the completion task of the knowledge graph is divided into three sub-tasks of head entity completion, relation completion, and tail entity completion. Head entity completion refers to when giving the relation and tail entity in the triple, we need to give head entities that can form reasonable triples with them. For example, give the relation "state of" and the tail entity "U.S.A", the possible head entity of the condition can be "California" or "Texas". The relation completion and tail entity completion are the same. It can be seen that in the completion task, the entity or relation that can constitute a triple is not unique.

It is not difficult to use the trained PTransD model for knowledge graph completion tasks. Taking the tail entity completion task as an example, for a triplet $T = (h, r, ?)$ whose tail entity is missing, we need to find a suitable tail entity t so that T becomes a valid triplet. Let $e_1, e_2, \cdots, e_n$ represent the n entities of the knowledge graph, and put them one by one into the missing position of T to form candidate triplets, denoted as $T_i = (h, r, e_i)$. Through the scoring function (12), the PTransD model gives the scores of the n candidate triples. After that, the top k candidate triples with the highest scores is taken as the model completion results, where k is a manually set parameter.

IV. Experiments and Results Analysis

In this section, we illustrate our experimental result of knowledge graph completion with the PtransD model.

A. Dataset

For the experimental data set, the public data set FB15k for validation of the translation model effect. The FB15k dataset is the largest commonly used single-language knowledge graph studied in recent years [3] [4] [5] [6] [7]. It contains about 15,000 entities from Freebase [2] and related triples. The detailed statistics of this data set are shown in Tab. I.

TABLE I
FB15k data set statistics

# Relation	# Entity	# Train	# Valid	# Test
1345	14951	483142	50000	59071

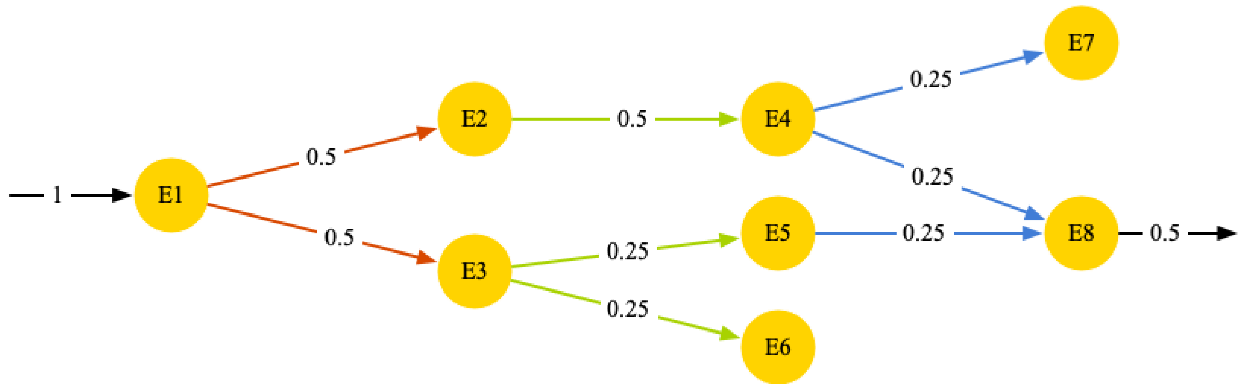

Fig. 2. An example for calculating relation path's reliability. Entities are represented by yellow dots and numbered from 1 to 8. Three kinds of relation r_1, r_2 and r_3 are displayed with red, green and blue arrows, respectively. When calculating the reliability of the relation path $p = (r_1, r_2, r_3)$ between E_1 and E_8, we assign 1 unit of resource to E_1 and make the resource flow along the graph. Finally, we'll obtain 0.5 unit of resource at E_2, which means the reliability of p is 0.5.

B. Experiments

In the experiment, the FB15k dataset is selected to evaluate the PTransD model on the knowledge completion task. The evaluation of the model is completed in three sub-tasks: i) head entity completion, ii) relation completion, and iii) tail entity completion. For each sub-task, the results of three indicators, Mean Rank, MRR [9], and Hits@10, are given. Mean Rank is the mean of correct entities' or relations' rank among the completion result. The MRR indicator calculates the mean value of ranks' reciprocal. Hits@10 indicates the proportion of valid entities or relations ranked in the top-10. In addition, we also calculate the averages of the head entity completion and tail entity completion on these three indicators, as the model's overall completion evaluation criteria. Literature [3] and [4] summarize the results of common existing model evaluations, and this paper refers to some of the results as a comparison of this model.

When training the PTransD model, we used the mini-batch SGD optimizer to optimize the loss function (13). The 2-norm of the entity vector, the relationship vector, and each projection vector is also limited to 1 to prevent the model from obtaining a trivial solution by increasing the norm. All the parameters of the PTransD model are initialized randomly. Corrupt triplet used for training is generated by replacing the head entity or the tail entity of the relation path. We found that there is a large number of relations among entities. In the dataset FB15k, the number of 2-hop relation paths is more than one hundred million while the 3-hop relation path's amount is more than 60 times more. It's very time consuming to consider all the relation paths between certain two entities. To reduce the amount of calculation, we limited the maximum length of the relation path to 2. The confidence of each path was calculated through the train set before training. We also discarded the path whose reliability is less than 0.01 to speed up the training process.

The PTransD model was verified on FB15k using multiple parameters. The batch size was fixed to 4800 and the maximum training epoch was set to 500. The average loss of model's completion on the validation set of FB15k was used as the basis of the early stop. The best result occurs when setting the margin to 1, the embedding dimension to 100, and the learning rate to 0.01, see Tab. II for details. Tab. III shows the detailed evaluation results of our model together with other models in FB15k.

TABLE II
EVALUATION RESULS OF PTRANSD IN FB15K

Task	Mean Rank	MRR	Hits@10%
head	190	0.266	50.4
relation	3	0.773	96.9
tail	189	0.271	54.6
total	189	0.268	52.5

TABLE III
EVALUATION RESULTS IN FB15K

Model	Mean Rank	Hits@10%
TransE [5]	243	34.9
TransH(bern) [6]	212	45.6
TransR(bern) [7]	198	48.2
TransD(bern) [4]	194	**53.4**
PTransE(ADD,2-STEP) [3]	200	51.8
PTransD(our)	**189**	52.5

Compared with common existing models, the PTransD model in the FB15k data set has a lower Mean Rank than TransD, and similar to the optimal result among these models on Hits@10, which shows that PTransD is effective in considering multi-step relation and embedding schemes for entities and relations. However, because the PTransD model can learn a richer relation between two entities from the relation path, its performance in accurately predicting missing entities or relations is lower than that of the TransD model, so its performance is slightly insufficient on the Hit@10 indicator.

V. Conclusion and Future Work

This paper explores the application of representation learning in knowledge graphs, focusing on the effects of translation models on knowledge graph completion. We introduce common translation models and compares the advantages and disadvantages of different models. Inspired by the construction ideas of the PTransE model and TransD, we proposed a translation model PTransD based on relational paths and dynamic projection. The PTransD model is a generalization of the TransD model. When the relation path length is limited to 1 and the reliability of the relation path is not taken into consideration,, the PTransD model is converted into a form in which the TransD model has the same dimensions in the entity space and relation space. Compared with the PTransE model, the proposed model embeds entities and relationships into different spaces, and projects entities into the relationship space dynamically according to the relations and entities themselves, thereby making the model more expressive. We verified the completion effect of the PTransD model in the benchmark dataset FB15k. The result indicates the rationality of PTransD for multi-step relations.

There is still much work to do for further research. At present, our work is based on the Trans series of models. These models are based on the structure and learning of the knowledge graph, but the semantic information in the knowledge graph is not only included in the structure, but also the text itself. Our follow-up work will focus on how to use the information in the knowledge graph to complete the knowledge graph completion problem.

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