Knowledge Graph Embedding with Multiple Relation Projections

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Abstract—Knowledge graphs contain rich relational structures of the world, and thus complement data-driven machine learning in heterogeneous data. One of the most effective methods in representing knowledge graphs is to embed symbolic relations and entities into continuous spaces, where relations are approximately linear translation between projected images of entities in the relation space. However, state-of-art relation projection methods such as TransR, TransD or TransSparse do not model the correlation between relations, and thus are not scalable to complex knowledge graphs with thousands of relations, both in computational demand and in statistical robustness. To this end, we introduce TransF, a novel translation-based method which mitigates the burden of relation projection by explicitly modeling the basis subspaces of projection matrices. As a result, TransF is far more light-weight than the existing projection methods, and achieves state-of-the-art performance. Especially, TransF improves by 9%/5% in the head/tail entity prediction task for N-to-1/to-N relations and achieves state-of-the-art performance. An effective solution is to consider two separate embedding spaces for entities and relations. Entities are then mapped into the relation space using relation-specific projections, such as those in TransR [14]. This mapping strategy, however, causes critical drawbacks. First, when the number of relations is large, the whole projection matrices are expensive to model. Second, treating each relation separately does not account for the latent structure in the relation space, leading to waste of resources. An example of such a latent structure is the correlation between relations “nationality” and “place-of-birth”, as the latter may infer about the former.

To this end, we propose a new translation-based method called TransF, which is inspired by TransR, but does not suffer from these problems. Under TransF, projection matrices are members of a matrix space spanned by a fixed number of matrix bases. A relation-specific projection matrix is characterized by a relation-specific coordinate in the space. Put in other way, the relation projection tensor is factorized into product of a relation-specific coordinate matrix and a basis tensor. Hence, TransF is much more efficient and robust than TransR. Fig. 1 illustrates the idea behind TransF.

We evaluate our TransF on the common link prediction task using two popular KGs: Freebase and WordNet. The experimental results show that TransF delivers significant improvements over state-of-the-art translation-based methods.

I. INTRODUCTION

Current data-driven machine learning works well in an homogeneous domain, but may not scale to domains that demand heterogeneous knowledge about entities and relations. Knowledge graphs (KGs), which encompass rich information about structures of the world, offer a complementary approach. Knowledge-augmented machine learning thus holds a promise to improve performance through knowledge reuse and to enable explanability [22]. These benefits have been found in many applications, ranging from vision [16], recommendation [9], question answering [5, 17, 10] to language modeling [11]. Despite huge efforts spent to build large-scale KGs such as Freebase [3], YAGO [22] or DBpedia [2], a major problem consistently remains: they are far from complete. Thus, it poses a canonical task of automatic completion from the existing knowledge base, which amounts to reasoning about unknown relations between entities.

A typical KG is represented as a graph whose nodes are entities and edges are relations between heads and tails. While this raw representation is adequate to store known knowledge, relating distant entities requires expensive graph traversal, possibly through multiple paths. Thus, knowledge graph completion calls for learning of a new representation that supports scalable reasoning. The most successful approach thus far is through embedding entities and relations into a continuous vector space, which naturally lends itself to simple algebraic manipulations [8]. A well-known method is TransE [6], which embeds entities and relations into the same space where the difference between head and tail is approximately the relation. While this embedding permits very simple translation-based relational inference, it is too restrictive in dealing with 1-to-N, N-to-1 and N-to-N relations.

An effective solution is to consider two separate embedding spaces for entities and relations. Entities are then mapped into the relation space using relation-specific projections, such as those in TransR [14]. This mapping strategy, however, causes critical drawbacks. First, when the number of relations is large, the whole projection matrices are expensive to model. Second, treating each relation separately does not account for the latent structure in the relation space, leading to waste of resources. An example of such a latent structure is the correlation between relations “nationality” and “place-of-birth”, as the latter may infer about the former.

To this end, we propose a new translation-based method called TransF, which is inspired by TransR, but does not suffer from these problems. Under TransF, projection matrices are members of a matrix space spanned by a fixed number of matrix bases. A relation-specific projection matrix is characterized by a relation-specific coordinate in the space. Put in other way, the relation projection tensor is factorized into product of a relation coordinate matrix and a basis tensor. Hence, TransF is much more efficient and robust than TransR. Fig. 1 illustrates the idea behind TransF.

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II. PRELIMINARIES

Let us first define common notations. A knowledge graph (KG) is constructed from a set of entities $\mathcal{E}$ and a set of relations $\mathcal{R}$. The basic unit representing a fact in KG is a triple, denoted as $(h, r, t)$ where $h$ is head entity, $r$ is relation and $t$ is tail entity. We use bold letters with normal font to indicate vectors and bold letters with capital font to indicate matrices. In this fashion, $h, r, t$ are the embedding vectors of $h, r, t$, respectively.

TransE: TransE [6] is a simple yet scalable and effective method for knowledge graph representation. It treats entities
The energy function now becomes:

$$E(h, r, t) = \|h + r - t\|_{1/2}$$

The energy should be low for true triples and high for incorrect triples. TransE performs well when relations are 1-to-1 but fails to handle relations of type 1-to-N, N-to-1 or N-to-N triples. TransH, on the other hand, adapt this commonness to specific relations. To solve this problem, TransH projects head and tail entities onto a relation–specific hyperplane before doing translation–based reasoning as in TransE. However, TransR introduces a huge number of additional parameters, causing poor robustness in learning and scalability issues for large KGs.

### III. Our Method: TransF

#### A. Correlation Among Relations.

In several knowledge bases such as Freebase, relations are organized in hierarchies. Relations belonging to the same subtree (e.g. containing similar prefixes) are correlated. Most relationships come from the semantic meaning of relations and some are partially independent of the entities. For example, in the FB15k dataset, two relations "/people/person/.../major_field_of_study" and "/people/person/placement_of_birth" and "/people/person/nationality" are highly dependent as the field of study is usually the main factor that affects the degree one can receive (e.g. Computer Science → Bachelor of Computer Science). Note that, in this case, we do not need any information about the head entity (a particular person) to decide this correlation. Another example is the pair of relations "/people/person/place_of_birth" and "/people/person/nationality" where a person born in New York is likely to have the United States nationality. Therefore, we argue that better modeling of correlations among relations will lead to more accurate representation of knowledge graphs.

#### B. TransF

Motivated from the above observation, we now present TransF, a new translation–based embedding method of knowledge graphs. Our model defines two factorized projection matrices as follows:

$$M_{r,h} = \sum_{i=1}^{s} \alpha_r^{(i)} U^{(i)} + I \quad (2)$$

$$M_{r,t} = \sum_{i=1}^{s} \beta_r^{(i)} V^{(i)} + I \quad (3)$$

where $s \in \mathbb{R}$ is the number of factors; $U^{(i)}, V^{(i)} \in \mathbb{R}^{d_r \times d_r}$ are relation space bases for projecting head and tail entities, respectively; $\alpha_r^{(i)}$ and $\beta_r^{(i)}$ are the corresponding coefficients of $U^{(i)}$ and $V^{(i)}$ characterized by the relation $r$. $I$ is the identity matrix, which serves as the base case when projections are not needed. It also provides a way to initialize TransF from TransE.

With this formulation, the underlying relationships among relations are explicitly encoded in the relation space bases \{U^{(i)}| i | \{1,s\}\} and \{V^{(i)}| i | \{1,s\}\}. $\alpha_r^{(i)}$ and $\beta_r^{(i)}$ on the other hand, adapt this commonness to specific relations. To deal with 1-to-N and N-to-1 relations, we project head and tail entities into spaces described by $M_{r,h}$ and $M_{r,t}$, respectively:

$$h_\perp = M_{r,h} h, \quad t_\perp = M_{r,t} t$$

Since $M_{r,h}$ and $M_{r,t}$ are factorized, each entity is now associated with multiple yet specific views rather than a single...
Statistics of datasets used in the experiments.

| Dataset   | #Train | #Valid | #Test | #Ent | #Rel |
|-----------|--------|--------|-------|------|------|
| FB15k     | 483,142| 50,000 | 59,071| 14,951| 1,345|
| FB15k-237 | 272,115| 17,535 | 20,466| 14,541| 237  |
| WN18      | 141,442| 5,000  | 5,000 | 40,943| 18   |
| WN18RR    | 86,835 | 3,303  | 3,134 | 40,943| 11   |

general view as in TransR. The energy function is similar to Eq. [1]. To avoid trivial solution (e.g. all embedded vectors are zeros) when minimizing the energy, we impose the following constraints in our model: \( ||h||_2 = ||t||_2 = 1, ||r||_2 \leq 1 \).

**Training loss:** We define the following margin-based loss function:

\[
\mathcal{L} = \sum_{(h,r,t) \in T} \sum_{(h',r',t') \in T'} [E(h, r, t) + \gamma - E(h', r', t')]_+
\]

where \([x]_+\) denotes max(0, x), \(\gamma\) is the margin, \(T\) is the set of positive triples and \(T'\) is the set of negative triples. Since the collection of all negative triples is huge, we need to focus on negative triples which are close to the correct ones. Similar to [6], given each correct triple \((h, r, t)\) sampled during training, we generate a negative example by replacing either head or tail entities but not both. Thus, the form of \(T'\) is:

\[
T' = \{(h', r, t) | h' \in E\} \cup \{(h, r', t') | t' \in E\} \forall (h, r, t) \in T
\]

We apply “bern” sampling trick suggested in [26] when corrupting triples to reduce the false-negative rate. In this setting, the probability of sampling head and tail entities are not equal but depends on relation types. For each relation \(r\), denote \(hpt\) as the average number of head entities per tail entity and \(tph\) as the number of tail entities per head entity. Then, given a triple \((h, r, t)\), the probability of corrupting \(h\) and \(t\) is \(\frac{hpt}{hpt+tph}\) and \(\frac{tph}{hpt+tph}\), respectively.

**IV. Experiments and Results**

**A. Datasets.**

For our experiments, we use two common datasets FB15k and WN18 [6] and their corresponding updated version FB15k-237 [23] and WN18RR [11]. According to [11], FB15k-237 and WN18RR do not contain reversible relations like FB15k and WN18, thus, are more difficult for link prediction task. Statistics of the datasets are provided in Table 1.

**B. Link Prediction.**

Given a test triple \((h, r, t)\) with either \(h\) or \(t\) is missing, our target is to complete this triple by finding the correct entity. Similar to [6], we formalize this task as a ranking problem. First, we replace the missing entity with every entity in the knowledge graph and compute the energy of each candidate triple in turn using Eq. [1]. Next, we filter out all correct triples in the knowledge graph different from the target one. Finally, we rank the energy values over the remaining triples in ascending order and use those ranks to decide which entity is the most suitable.

We used grid search for hyper-parameter tuning with the margin \(\gamma\) is among \{1, 2, 4\}, the size of entity embedding \(d_e\) and relation embedding \(d_r\) are among \{20, 50, 100, 150, 200\}, the number of relation space bases \(s\) is among \{3, 5, 10, 15\}. The optimizer is Adam [13] with the learning rate \(\lambda\) of 0.001. Following other papers, we pretrained our model with TransE by setting the relation coefficients to 0 for 1000 epochs then continued training for a maximum of 150 epochs. The optimal settings of our model on the validation set are \(\gamma = 4, d_e = d_r = 50, s = 5\) for WN18 and WN18RR, \(\gamma = 2, d_e = d_r = 150, s = 5\) for FB15k and \(\gamma = 4, d_e = d_r = 100, s = 5\) for FB15k-237.

There are three evaluation metrics for this task: (i) Mean Rank (MR) (ii) Mean Reciprocal Rank (MRR) and (iii) Hits@10. A better model would expect lower MR and higher MRR/Hits@10. The overall results are shown in Table 1. TransF outperforms all translation-based models by a large margin on WN18 and FB15k, achieving the best results on all evaluation metrics. Compared to methods belonging to other disciplines, TransF also demonstrates good performance with the best MR (3246) on WN18RR and the best Hits@10 (47.2%) on FB15k-237. It suggests that factorizing the relation space as a combination of multiple sub-spaces is critical for representing different types of relations in knowledge graphs. This statement is further supported when looking at Table 3. For 1-to-1 and N-to-N relations, TransF produces higher accuracy than all baseline models in both HEP and TEP. Specifically, for HEP with N-to-1 relations and TEP with 1-to-N relations, our model improves the results by about 9% and 5% over the second best model TransSparse (us), respectively.

**C. Relation Representation with TransF.**

In Fig. 2, we show the t-SNE visualization of all relations in FB15. There are three main things to note here: (i) Our model successfully captures the correlations among relations as relations with similar semantic meaning usually stay close in the embedded space. (ii) Correlated relations do not necessarily belong to the same category but can span across different categories. For example, in group 4 two relations “base/schemastaging/...team” and “/sports/pro_athlete/...team” are from two categories “base” and “sports”, respectively. (iii) Although most information of a relation is stored in the translation vector due to its large size, the coefficient vectors also provide certain amount of information to make the relation representation more accurate. As in Fig. 2, when relation representation does not contain coefficient vectors, the relations in group 1 and 2 seem to merge together even though they are not very similar. On the other hand, when coefficient vectors are used, these two groups are more separately.

**D. Complexity Analysis of TransF.**

In Fig. 3, we plot the number of parameters and training time of TransF in comparison with some other translation-based
Table II

| Method   | WN18  | FB15k | WN18RR | FB15k-237 |
|----------|-------|-------|--------|-----------|
|          | MR    | MRR   | Hits@10 | MR        | MRR   | Hits@10 | MR    | MRR   | Hits@10 | MR    | MRR   | Hits@10 |
| TransE   | 251   | -     | 89.2    | 125       | -     | 47.1    | -     | -     | -       | -     | -     | -       |
| TransH   | 388   | -     | 82.3    | 87        | -     | 64.4    | -     | -     | -       | -     | -     | -       |
| TransR   | 225   | -     | 92.0    | 77        | -     | 68.7    | -     | -     | -       | -     | -     | -       |
| CTransR  | 218   | -     | 92.3    | 75        | -     | 70.2    | -     | -     | -       | -     | -     | -       |
| TransD   | 212   | -     | 92.2    | 91        | -     | 77.3    | -     | -     | -       | -     | -     | -       |
| TransSparse (s) | 221  | -   | 92.8   | 82        | -     | 79.5    | -     | -     | -       | -     | -     | -       |
| TransSparse (us) | 211 | - | 93.2 | 82 | - | 79.9 | - | - | - | - | - | - |

*: The result of DistMult and Complex on WN18RR and FB15k-237 are taken from [11].

Table III

| Method   | Head Entity Prediction (HEP) | Tail Entity Prediction (TEP) |
|----------|-------------------------------|-------------------------------|
|          | 1-to-1 | 1-to-N | N-to-1 | N-to-N | 1-to-1 | 1-to-N | N-to-1 | N-to-N |
| TransE   | 43.7   | 65.7   | 18.2   | 47.2   | 43.7   | 19.7   | 66.7   | 50.0   |
| TransH   | 66.8   | 87.6   | 28.7   | 64.5   | 65.5   | 39.8   | 83.3   | 67.2   |
| TransR   | 78.8   | 89.2   | 24.1   | 69.2   | 79.2   | 37.4   | 90.4   | 72.1   |
| CTransR  | 81.5   | 89.0   | 34.7   | 71.2   | 80.8   | 38.6   | 90.1   | 73.8   |
| TransD   | 86.1   | 95.5   | 39.8   | 78.5   | 85.4   | 50.6   | 94.4   | 81.2   |
| TransSparse (s) | 86.8 | 95.5 | 44.3 | 80.9 | 86.6 | 56.6 | 94.4 | 83.3 |
| TransSparse (us) | 87.1 | 95.8 | 44.4 | 81.2 | 87.5 | 57.0 | 94.5 | 83.7 |

Figure 2. tSNE visualization of all relations in FB15k. For each relation \( r \), the representation vector is constructed by concatenating the translation vector \( r \) and two coefficient vectors \( \alpha_r \) and \( \beta_r \) into a single vector. Some related relations are highlighted in red and are grouped together. To better understand the meaning of these relations, they are zoomed with names. The small rectangle snapshot marked with * is the tSNE embedding of relations in group 1 and 2 by using the translation vector \( r \) only.
methods on FB15k. When the number of space bases \( s \) is small, TransF has nearly the same number of parameters as TransE and TransH. Increasing \( s \) only grows the number of parameters by a small constant rate. Not only consuming fewer parameters, TransF also runs faster than TransR and TransD. Specifically, with \( s=5 \), TransF can be trained in roughly half amount of time compared to TransR. This difference reduces to about 20% when \( s = 100 \). In this experiment, we also observe an unexpected pattern: TransD is slower than TransR though its projection matrix is factorized as product of two vectors. This is because TransD has to recompute its projection matrix for every triple while TransR can index its projection matrix based on relations. Our method does not suffer this problem, hence, is much more efficient than TransD. However, the training time of TransF is still not comparable to TransE and TransH. It explains why pretraining with TransE is necessary.

V. RELATED WORK

**Translation based methods:** Beside TransE, H, R, D, Sparse that we have already discussed, there are other models falling into this category. **lppTransD** [29] is an extension of TransD that accounts for different roles of head and tail entities. This idea is also applied in our model as we use two separate sets of basis matrices \( \{U(i)\} = I, \{V(i)\} = I \) to compute the projection matrices for head and tail entities. **STransE** [18] combines Structured Embedding (SE) [7] and TransE into a single model. Its energy function is \( E(h, r, t) = \| W_r h + W_r t \|_{\ell_2} \). In fact, this model is similar to lppTransR [29]. **KB2E** [12] takes an interesting approach to handle non-injective relations by incorporating knowledge graph uncertainty into embedding. Specifically, it models entities and relations as Gaussian distributions instead of single points in the embedding space: \( x \sim N(\mu_x, \Sigma_x) \) for \( x = h, t, r \). The KL divergence between two distributions \( h - t \) and \( r \) is selected to be an (asymmetric) energy function very naturally: \( E = D_{KL}(h - t, r) = D_{KL}(N(\mu_h - \mu_t, \Sigma_h + \Sigma_t), N(\mu_r, \Sigma_r)) \).

**Tensor based methods:** Tensor based methods represent a knowledge graph as a 3D tensor \( \chi \) of shape \( N_e \times N_e \times N_r \) where \( N_e \) and \( N_r \) are the number of entities and relations in the knowledge graph, respectively. Each element \( \chi_{ijk} \) of the tensor can be seen as probability that the triple \((e_i, r_k, e_j)\) is correct.

**RESCAL** [20] applies tensor factorization to estimate \( \chi \). Specifically, each slice matrix \( \chi_{:,ik} \) (\( k = 1, N_r \)) along the relation axis is computed as \( \chi_{:,ik} = E R_k E^t \) where \( E \in \mathbb{R}^{N_e \times s} \) is a latent factor matrix of the entities, \( R_k \in \mathbb{R}^{s \times s} \) is an matrix that models the interactions of the components with respect to the \( k \)-th relation. Compared to TransE with the same number of hidden units, RESCAL requires far more parameters (as much as TransR). In addition, the three-way dot product make this model more difficult to be trained. This is the reason why RESCAL is not comparable to TransE in many situations [6].

**DistMult** [28] is a simplified version of RESCAL with the energy function \( E(h, r, t) = \| h W_r^t \|_1 \). Here, the interaction between head and tail entities is captured via a diagonal matrix \( W_{diag} \) instead of a 3D tensor like in NTN. In fact, we can rewrite the energy function of DistMult as \( E(h, r, t) = \sum(h \circ r \circ t) \) where \( r \in \mathbb{R}^{d_e} \) is the main diagonal of \( W_{diag} \). In this form, DistMult looks very similar to TransE but with additive operators replaced by multiplicative ones.

**Holographic Embedding (HolE)** [19], a novel method leveraging the holographic models of associative memory to learn the compositional representations of knowledge graphs. The probability of a triple \((e_i, r_k, e_j)\) to be correct is computed as: \( \chi_{ijk} = \sigma(\phi_{i,j,k}) = \sigma(r_k^t (e_i \circ e_j)) \) where \( \phi_{i,j,k} \) is a characteristic function over the triple, \( r_k \in \mathbb{R}^{d_e} \) are the relation and entity embeddings; \( \sigma \) is a circular correlation operator. From the holography angle [21], we can see that the association of \( r_k \) and \( e_i \) is, first, implicitly stored in \( e_j \) via training. Then, taking a circular correlation with \( e_i \), will return \( r_k \) - a noisy version of \( r_k \). And finally, the dot product with \( r_k \) will examine how similar this two vectors are. HolE has many advantages such that computation efficiency (only calculating on vectors), scalability (the number of parameters is small) and capability of representing anti-symmetric relations (\( \ast \) is non-commutative).

Another model closely related to HolE is **Complex Embedding (ComplEx)** [25]. It originates from the observation that embedding relations and entities into complex spaces would be better than into real spaces due to the non-symmetry of the Hermitian product. The characteristic function \( \phi_{i,j,k} \) of ComplEx is defined as: \( \phi_{i,j,k} = Re(\langle r_k, e_i, e_j \rangle) \) where \( r_k, e_i, e_j \) are complex vectors; \( \langle a, b, c \rangle \) is a trilinear product between \( a, b, c; \overline{a} \) is the conjugate of \( a \). ComplEx and HolE have been proven to be mathematically equivalent [24]. Thus, both models provide the same representation power.

**Other related methods:** One early work that applied the embedding concept for knowledge graph completion is **Structured Embedding (SE)** [7]. The basic idea of this model is that two entities of a correct triple should be close to each
other in some relation spaces. Hence, its energy function is defined as $E(h, r, t) = \|W_{r,t}h - W_{r,t}v\|_{\ell_2}$.

**Semantic Matching Energy (SME)** introduces the relation embedding $r$ and treats it equally to the entity embeddings $h$ and $t$. This method is suitable for situations when relations and entities are interchangeable, for example, in NLP, a verb typically corresponds to a relation but sometimes can also be an entity. SME defines the energy function as $E(h, r, t) = -f(h, r)\cdot g(t, r)$ where $f$ and $g$ are neural networks. In case $f$ and $g$ are linear, this energy function only captures two-way interactions of pairs $(h, r)$, $(t, r)$ and $(h, t)$ rather than the three-way interaction as in RESCAL.

Both SE and RESCAL can be seen as special cases of **Neural Tensor Network (NTN)** whose energy function is $E(h, r, t) = u_r^T \sigma(W_{r,h}^T h + U_r h + V_r t + b)$ where $\sigma$ is a nonlinear activation function (e.g. $\tanh$), $W_{r,h} \in \mathbb{R}^{d_r \times d_h \times k}$, $U_r, V_r \in \mathbb{R}^{d_r \times k}$ and $u_r \in \mathbb{R}^k$ all depends on $r$. Despite being expressive. NTN does not scale well to knowledge graphs with large number of relations (e.g. FB15k) due to its high computational cost.

**VI. Conclusion**

We have proposed TransF, a new knowledge graph embedding method explicitly models the relationship between relations. Our model decomposes the relation–specific projection spaces into a small number of spanning bases, which are shared by all relations. We showed that this strategy not only leads to better performance but is also more efficient than state-of-the-art translation-based methods like TransR or TransD through extensive experiments on link prediction and complexity analysis. In addition, the visualization of learnt relations also indicates that TransF models the relation correlations well. In the future, we plan to explore better representation of relations. One potential way is using additional information from larger structures such as paths or subgraphs instead of triples only. Another direction is to define class–specific model of relations.

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