SpaceE: Knowledge Graph Embedding by Relational Linear Transformation in the Entity Space

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ABSTRACT
Translation distance based knowledge graph embedding (KGE) methods, such as TransE and RotateE, model the relation in knowledge graphs as translation or rotation in the vector space. Both translation and rotation are injective; that is, the translation or rotation of different vectors results in different results. In knowledge graphs, different entities may have a relation with the same entity; for example, many actors starred in one movie. Such a non-injective relation pattern cannot be well modeled by the translation or rotation operations in existing translation distance based KGE methods. To tackle the challenge, we propose a translation distance-based KGE method called SpaceE to model relations as linear transformations. The proposed SpaceE embeds both entities and relations in knowledge graphs as matrices and SpaceE naturally models non-injective relations with singular linear transformations. We theoretically demonstrate that SpaceE is a fully expressive model with the ability to infer multiple desired relation patterns, including symmetry, skew-symmetry, inversion, Abelian composition, and non-Abelian composition. Experimental results on link prediction datasets illustrate that SpaceE substantially outperforms many previous translation distance based knowledge graph embedding methods, especially on datasets with many non-injective relations. The code is available based on the PaddlePaddle deep learning platform https://www.paddlepaddle.org.cn/.

KEYWORDS
Knowledge Graph Embedding, Link Prediction, Non-Injective Relations

1 INTRODUCTION
Extracting entities and relationships from web texts [3, 9, 22, 35–37, 42, 44, 47, 49] and reasoning using the extracted information [8, 25] is the long-term goal of data-mining and natural language processing. From the philosophy of representation learning, entities and relations (either natural texts or symbols) can be represented by embedding representations, and the reasoning can be performed by applying the mathematical operations on these embedding vectors. This methodology has been successfully applied in the field of knowledge graph embedding in both symbolic knowledge-bases [6, 38, 46] and open-domain textual fact corpus [12], for the applications of knowledge graph completion [27], question answering [13], topic modeling [20] and so on.

The core theoretical problems of this methodology are to find appropriate embedding form and the mathematical operation for reasoning. These problems have been mostly studied in the field of knowledge graph embedding for the task of knowledge graph completion. The background of knowledge graph completion is that: although the large scale knowledge graphs such as Yago [34] and Freebase [5] store vast amounts of fact triples about the relationships between entities, knowledge graphs are incomplete and have missing relationships between entities. As the facts in knowledge graphs can be represented by (head, relation, tail) and (? , relation, tail) knowledge graph embedding (KGE) methods learn embedding representations of the entities and relations and use distance score functions to measure the plausibility of candidate fact triples. There are three major types of KGE methods: Translation distance-based methods model the relations as geometric transformations from the head entity vector to the tail entity vector and use norms as the score functions; Bilinear
The task of link prediction in knowledge graphs has been extensively studied in the literature, and many methods have been proposed. Traditional approaches use rule-based logics [31], or collect path features and use logistic regression on the features [18, 19] for link prediction. Knowledge graph embedding methods later become popular given their simplicity, scalability, and better performance than traditional approaches. A few recent studies [30, 48] combine the rule-based Markov Logic Networks (MLNs) and knowledge graph embedding methods and achieve promising results. We briefly review some knowledge graph embedding methods and discuss their connections to our work.

2 RELATED WORK

The task of link prediction in knowledge graphs has been extensively studied in the literature, and many methods have been proposed. Traditional approaches use rule-based logics [31], or collect path features and use logistic regression on the features [18, 19] for link prediction. Knowledge graph embedding methods later become popular given their simplicity, scalability, and better performance than traditional approaches. A few recent studies [30, 48] combine the rule-based Markov Logic Networks (MLNs) and knowledge graph embedding methods and achieve promising results. We briefly review some knowledge graph embedding methods and discuss their connections to our work.

Translation Distance Based Methods. TransE [6] represents entities and relations as vectors and models the relation as a translation from the head entity to the tail entity, i.e., vec(head)+vec(relation) = vec(tail). Along the line, TorusE [11] and RotatE [38] are proposed to model relation as translation on a compact Lie group and rotation in a complex vector space, respectively. The relational operations in previous translation distance based methods are injective. The non-injective property of relations is discussed in several extensions of TransE, such as TransH [43] and TransR [21]. They project the vectors of entities into a subspace and then perform relational translation between entities in the subspace. Different entity vectors of non-injective relations could be the same in the subspace. Despite the capability of these methods to model non-injective relations, their overall performance on benchmark datasets lags behind the recent state-of-the-art methods such as RotatE [38] and ConvE [10], and they can only model part of the relation patterns. MQuadE [46] addresses the problem of learning the non-injective relationships using a quadruple matrix representation for fact triples, in which the entity embedding matrices are required to be symmetric. The MQuadE has good theoretical properties and performs well in real-world tasks. Our proposed method - SpaceE has similar theoretical properties as MQuadE, and it does not impose symmetry on the entity embedding matrices (in fact, the entity embedding matrices are not necessarily square), which makes SpaceE more flexible and achieves comparable or even better performance than MQuadE in real-world tasks.

Bilinear Semantic Matching Methods. RESCAL [29] is the first bilinear model that uses matrices to represent relations. DistMult [45] simplifies RESCAL and employs a diagonal matrix for relation modeling. As DistMult uses a symmetric score function, it cannot model skew-symmetry relations. Trouillon et al. [41] proposed ComplEx to model skew-symmetry relations.

Deep Learning Methods. Neural networks such as neural tensor networks [33] and convolutional neural networks [10] were leveraged for knowledge graph completion. Although they have strong expressiveness, they lack the interpretability of relation reasoning. Moreover, the high performances of some recent neural network methods [26] can be attributed to the inappropriate evaluation protocols [39].

Tensor Decomposition Methods. The knowledge graph triples can be regarded as a 3-order tensor. Canonical Polyadic (CP) tensor decomposition is leveraged in Kazemi and Poole [15], Lacroix et al. [17] for knowledge graph completion. Balazevic et al. [2] proposed TuckER based on Tucker tensor decomposition. TuckER benefits from multi-task learning by sharing parameters through the core tensor.

3 RELATION MODELING BY LINEAR TRANSFORMATION

3.1 Notations

We use bold upper case letters to denote matrices. We denote the identity matrix as I, the Frobenius norm of a matrix A as ∥A∥F, the element-wise product of two matrices A and B as A ⊗ B, and the Hadamard product of two complex vectors a and b as a ◦ b.
3.2 The SpaceE Model

Let \( E = \{e_1, e_2, \cdots, e_n\} \) be the set of entities, \( \mathcal{R} = \{r_1, r_2, \cdots, r_m\} \) be the set of relations, and \( T = \{(h_i, r, t_i)\} \) be the collection of fact triples, where \( h_i \in E \) is the head entity, and \( t_i \in E \) is the tail entity, \( r_i \in \mathcal{R} \) is the relation.

SpaceE represents entities as \( p \times q \) matrices and relations as \( q \times q \) square matrices. Let \( H, R, T \) denote the matrix of the head entity \( h \), the relation \( r \), and the tail entity \( t \), respectively. SpaceE uses the following score function to measure the plausibility of a fact triple \((h, r, t)\):

\[
d(h, r, t) = \|HR - T\|_F^2.
\]

The idea behind the score function is that the relation between two entities corresponds to a linear transformation of entity matrices. It is expected that \( HR \approx T \) when the fact triple \((h, r, t)\) holds, while \( HR \) should be far away from \( T \) otherwise.

Since \((h, r, t)\) is equivalent to \((\hat{r}, \hat{h}, h)\) where \( \hat{r} \) is the reverse relation of \( r \), we can adopt the reciprocal learning approach [17] and develop following score function:

\[
f(h, r, t) = \|\hat{T}R - H\|_F^2,
\]

where \( \hat{R} \) is the representation of \( \hat{r} \). The score function \( d(h, r, t) \) is utilized for head entity prediction while the score function \( f(h, r, t) \) is utilized for tail entity prediction during training and inference. As a result, a tail entity may have many head entities when \( R \) is singular, and a head entity may have many tail entities when \( \hat{R} \) is singular. In other words, the non-projective property of relation is preserved. See Section 4 for more details.

3.3 Training

The training process samples a mini-batch of fact triples from training data and randomly corrupts the head entities and tail entities to obtain negative samples for head entity prediction and tail entity prediction, respectively. It optimizes a loss function to make the scores of true triples lower than that of negative triples. After training, the scores are utilized to rank candidate entities to answer the link prediction queries.

We use the self-adversarial negative sampling loss function [24, 38] to learn the parameters:

\[
\mathcal{L} = -\log \sigma(y - d(h, r, t)) - \log \sigma(y - f(h, r, t))
\]

\[
- \sum_{i=1}^{k} p(\hat{h}_i, r, t) \log \sigma(\hat{d}(\hat{h}_i, r, t) - y)
\]

\[
- \sum_{i=1}^{k} p(h, r, \hat{t}_i) \log \sigma(f(h, r, \hat{t}_i) - y),
\]

where \( \sigma \) is the sigmoid function, \( y \) is the fixed margin, \( \hat{h}_i \) is the \( i \)-th sampled negative head entity, and \( \hat{t}_i \) is the \( i \)-th sampled negative tail entity, \( p(\hat{h}_i, r, t) \) and \( p(h, r, \hat{t}_i) \) are the negative sample weights in the self-adversarial loss [38] defined as:

\[
p(\hat{h}_i, r, t) = \frac{\exp(\sigma(y - d(\hat{h}_i, r, t)))}{\sum_{j=1}^{k} \exp(\sigma(y - d(\hat{h}_j, r, t)))},
\]

\[
p(h, r, \hat{t}_i) = \frac{\exp(\sigma(y - f(h, r, \hat{t}_i)))}{\sum_{j=1}^{k} \exp(\sigma(y - f(h, r, \hat{t}_j)))}.
\]

where \( \alpha \) is the self-adversarial temperature. The weight corresponding to a negative sample is large when the model predicts the negative sample as a true fact triple.

The orthogonal constraint can stabilize the training and ease overfitting [4]. Orthogonal linear transformation has the nice property of preserving the norm. We propose a regularization term to encourage the relation matrix to be nearly orthogonal. Note that orthogonal matrices \( R^T R = I \) and they are non-singular. We design a regularization term \( \| (R^T R) \otimes (R^T R) - R^T R \|_F^2 \) to encourage the elements in \( R^T R \) to be either 1 or 0. The relation matrix satisfying the regularization constraint is nearly orthogonal and could be singular. The regularized loss function is

\[
\mathcal{L}_{reg} = \mathcal{L} + \lambda \left( (\| R^T R \|_F^2 - 1)^2 + (\| R^T R \|_F^2 - 1)^2 \right),
\]

where \( \lambda \) is the regularization hyper-parameter.

4 MODEL PROPERTY ANALYSIS

4.1 Infer Relation Properties

Theorem 4.1. SpaceE can model non-injective, symmetric, skew-symmetric, inversion, Abelian composition, and non-Abelian composition relations with different relation matrices, as summarized in Table 1.

| Relation Property | Relation Matrix |
|-------------------|----------------|
| Non-injective     | \( R \) or \( R \) is singular |
| Symmetric         | \( R^2 = I \) |
| Skew-symmetric    | \( R^2 \neq I \) |
| \( r_2 \) inversion of \( r_1 \) | \( R_1 R_2 = R_2 R_1 = I \) |
| \( r_3 = r_1 \otimes r_2 \) | \( R_1 \oplus R_2 = R_1 \oplus R_2 = I \) |
| \( r_1 \otimes r_2 \) Abelian | \( R_1 R_2 = R_1 R_2 = R_1 R_2 = R_1 R_2 = I \) |
| \( r_1 \otimes r_2 \) Non-Abelian | \( R_1 \otimes R_2 \neq R_1 \otimes R_2 \) |

Table 1: The ability of SpaceE to model various relation properties with different relation matrices.

Proof. **Non-injective Relation.** A relation \( r \) is non-injective, iff there exist multiple fact triples \( (h_i, r, t_i), \cdots, (h_k, r, t_k) \), where \( h_1, \cdots, h_k \) are different or multiple fact triples \( (h, r, t_1), \cdots, (h, r, t_k) \), where \( t_1, \cdots, t_k \) are different. In SpaceE, when \( R \) is singular, the equation \( XR = T \) can have different solutions \( X = H_1, \cdots, H_k \): when \( \hat{R} \) is singular, the equation \( Y \hat{R} = H \) can have different solutions \( Y = T_1, \cdots, T_k \).

**Symmetric Relation.** For a symmetric relation \( r \), for any two entities \( h, t \in E \), the fact triple \((h, r, t)\) holds \( \iff \) the fact triple \((t, r, h)\) holds. In SpaceE, it requires \( HR = T \iff TR = H \).

It follows from \( R^2 = I \).

**Skew-symmetric Relation.** For a skew-symmetric relation \( r \), for any two entities \( h, t \in E \), the fact triple \((h, r, t)\) is true \( \iff \) the fact triple \((t, r, h)\) is false. This requires in SpaceE that

\[
HR = T \iff TR \neq H.
\]
It follows from $R^2 \neq I$.

**Inversion Relation.** A relation $r_2$ is the inversion of relation $r_1$ iff for any two entities $h, t \in \mathcal{E}$, the fact triple $(h, r_1, t)$ is true $\iff$ the fact triple $(t, r_2, h)$ is true. It requires in SpaceE,

$$HR_1 = T \iff TR_2 = H.$$

It follows from $R_1R_2 = R_2R_1 = I$.

**Relation Composition.** A relation $r_3 = r_1 \otimes r_2$ is the composition of two relations $r_1$ and $r_2$ iff for any three entities $a, b, c \in \mathcal{E}$, the facts $(a, r_1, b), (b, r_2, c)$ are true $\iff$ the fact $(a, r_3, c)$ is true. This requires in SpaceE that

$$AR_1 = B, BR_2 = C \implies AR_3 = C.$$

It follows from $R_3 = R_1R_2$.

**Abelian Composition and Non-Abelian Composition.** Let $r_3 = r_1 \otimes r_2$ be the composition of the relation $r_1$ and $r_2$, $r_4 = r_2 \otimes r_1$ be the composition of the relation $r_2$ and $r_1$. In SpaceE, the matrix representations of the two composite relations $r_3$ and $r_4$ can be written as

$$R_3 = R_1R_2, \quad R_4 = R_2R_1.$$

When $R_1R_2 = R_2R_1$, the composition of $r_1$ and $r_2$ is Abelian; otherwise, the composition is non-Abelian.

### 4.2 Connection to RotatE

We show that our model SpaceE can be regarded as an extension of RotatE [38].

**Theorem 4.2.** SpaceE subsumes RotatE with the special block diagonal matrix representations of complex vectors.

**Proof.** RotatE uses complex vectors to represent entities and relations and models the relation between two entities as the rotation in complex vector space. The score function of a fact triple $(h, r, t)$ in RotatE is

$$s(h, r, t) = \|h \circ r - t\|, \quad |r_1| = 1,$$

where $h, r, t \in \mathbb{C}^{K}$ are complex vector representations of head entity, relation, tail entity respectively.

A complex number $z = a + bi$ can be represented by a $2 \times 2$ matrix $\begin{pmatrix} a & -b \\ b & a \end{pmatrix}$. The product of two complex numbers $z_1 = a + bi$ and $z_2 = c + di$ is $z_1z_2 = ac - bd + (bc + ad)i$, which corresponds to the product of two matrices:

$$\begin{pmatrix} a & -b \\ b & a \end{pmatrix} \begin{pmatrix} c & -d \\ d & c \end{pmatrix} = \begin{pmatrix} ac - bd & ad - bc \\ bc + ad & bd + ac \end{pmatrix}.$$

A complex vector $z = (z_1, z_2, \ldots, z_K) \in \mathbb{C}^{K}$ can be represented as a $2K \times 2K$ block diagonal matrix $Z = \text{diag}(Z_1, Z_2, \ldots, Z_K)$ whose $i$-th block component $Z_i$ is the $2 \times 2$ matrix representation of $z_i$. Let $z, s \in \mathbb{C}^{K}$ be two complex vectors and $Z, S$ be their corresponding block diagonal matrices respectively. The Hadamard product of $z$ and $s$ is

$$z \odot s = (z_1s_1, z_2s_2, \ldots, z_Ks_K).$$

It is equivalent to the product of matrices $Z$ and $S$,

$$ZS = \text{diag}(Z_1S_1, Z_2S_2, \ldots, Z_KS_K).$$

As a result, the score function of RotatE corresponds to the score function of SpaceE if we change the complex vector representations of entities and relations to the corresponding block diagonal matrix representations.

### 4.3 Time and Space Complexity

RotatE and TransE use vectors of dimension $n$, the time and space complexity is $O(n^2)$. SpaceE uses $p \times q$ and $q \times q$ matrices for entity and relation representations, respectively. Its space complexity is $O(pq + q^2)$; its time complexity is $O(q^2)$. Assume that there are $n_e$ entities and $n_r$ relations, the total number of parameters in SpaceE is $n_e pq + n_r q^2$. In experiments, we set $p \approx \sqrt{n_r}, q = \sqrt{n}$ and use the number of parameters not more than RotatE for a fair comparison. For example, in the FB15k dataset, RotatE uses 1000 dimensions complex vectors; it has 20000 parameters of a complex vector; 1000 for the real part, 1000 for the imaginary part. SpaceE uses $45 \times 45 = 2025$ dimensions embedding matrices. In the Yago3-10 dataset, RotatE has $500 \times 2 = 1000$ parameters in a complex vector; SpaceE has $20 \times 40 = 800$ parameters in an embedding matrix.

### 5 EXPERIMENTS

#### 5.1 Experimental Setup

**Datasets.** We conduct experiments on five benchmark datasets: FB15k, WN18, FB15k-237, WN18RR, and YAGO3-10. The statistics of the datasets are summarized in Table 2.

FB15k [6] is a subset of FreeBase [5], a large-scale knowledge graph about the general world knowledge. FB15k samples 15k entities and their relations such as /location/country/capital from FreeBase.

WN18 [6] is a subset of the WordNet, a lexical database for the English language that groups synonymous words into synsets. WN18 contain relations between words such as hypernym and similar_to.

FB15k-237 [40] and WN18RR [10] are subsets of FB15k and WN18, respectively, with the inverse relation deleted to resolve the test set leakage problem and to examine the relation composition modeling ability.

YAGO3-10 [23] is a subset of YAGO3 whose entities have at least ten relations. Most of the relations in YAGO3-10 are descriptive attributes of people such as wasBornIn, worksAt, and graduatedFrom, which are non-injective. As shown in Table 2, the average number of head per tail of these relations is 913.

**Evaluation Metrics and Protocols.** We use the mean reciprocal rank (MRR) and HIT@1, 3, 10 as the metrics to evaluate different models. MRR measures the average of the inverse rank of correct entities in the list predicted by the model. HIT@k measures the average percentage of correct entities that are ranked in the top $k$ by the model. Following Bordes et al. [6], we use the filtered evaluation setting where the triplets that appear either in the training, validation, or test set (except the test triplet of interest) are removed from the list of corrupted triplets. To deal with the case that the
model may predict the same score for different fact triples, we adopt the random evaluation protocol suggested by Sun et al. [39].

**Baselines.** We compare our model with representative state of the art models, including distance translation based methods (TransE [6], SE [7], TransH [43], RotatE [38], BoxE [1]), bi-linear semantic matching methods (DistMult [45], ComplEx [41], TuckER [2]), and a deep learning method ConvE [10].

**Implementation Details.** The Adam optimizer [16] is utilized for model training. We tune the hyper-parameters with grid search and select the model that have highest MRR on the validation dataset. The hyper-parameters are selected from following configurations: the dimension of entity and relation matrices \( p, q \in \{10, 20, 40, 45\} \), the self-adversarial temperature \( \alpha \in \{0.5, 1.0\} \), the fixed margin \( \gamma \in \{3, 6, 9, 12, 24\} \), the number of negative samples \( k \in \{256, 512, 1024\} \), the regularization coefficient \( \lambda \in \{0.005, 0.01, 0.05, 0.1, 0.3, 0.6\} \), the batch size \( b \in \{512, 1024\} \), the initial learning rate \( lr \in \{1e-4, 2e-4\} \). The best hyper-parameters on each dataset are given in Table 3. The entity and relation matrix parameters are randomly initialized from the normal distribution \( \mathcal{N}(0, 0.01) \). Our algorithms are implemented on the PaddlePaddle deep learning framework https://www.paddlepaddle.org.cn/.

| Dataset    | #entity | #relation | #train | #valid | #test | #tphr | #hptr |
|------------|---------|-----------|--------|--------|-------|-------|-------|
| FB15k      | 14951   | 1345      | 483142 | 50000  | 59071 | 9.3   | 19.7  |
| WN18       | 40943   | 18        | 141442 | 5000   | 5000  | 4.2   | 4.2   |
| FB15K-237  | 14541   | 237       | 272115 | 17535  | 20466 | 7.9   | 65.9  |
| WN18RR     | 40943   | 11        | 86835  | 3034   | 3134  | 4.5   | 2.9   |
| YAGO3-10   | 123182  | 37        | 1079040| 5000   | 5000  | 3.5   | 913.1 |

Table 2: Statistics about the datasets. Among all the triplets of a relation \( r \), let \( tphr \) denote the average number of tail entities per head entity, \( hptr \) denote the average number of head entities per tail entity. \( #tphr \) denotes the average of \( tphr \) for all relations, \( #hptr \) denotes the average of \( hptr \) for all relations.

### 5.2 Main Results

We highlight the best results on the model category with a bold font and mark the best overall results by underlines in Tables 4, 5, 6.

Table 4 summarizes the results on the FB15k and WN18 datasets. The results of TransE are taken from later work’s implementation [28]. The results show that SpaceE can get comparative results on all the evaluation metrics with the state of the art baselines. TransH explicitly models non-injective relations but does not get overall competitive results. As discussed in Dettmers et al. [10], Sun et al. [38], many test triples in the two datasets appear as a reciprocal form of the training samples, and the test set leakage through inverse relation makes the datasets less challenging. The main relation patterns of the two datasets are symmetry, skew-symmetry, and inversion. The competitive performance of SpaceE demonstrates its capability to model the three relation patterns.

The difference between the results of RotatE and SpaceE is minor. This could be explained by our analysis of the connection between SpaceE and RotatE in Section 4.2.

From the results in Table 5, we observe that on FB15k-237, SpaceE achieves the best performance among the translation distance based knowledge graph embedding methods on all evaluation metrics. Its performance is competitive with the state-of-the-art semantic matching method TuckER, especially on Hits@10. The main relation pattern in FB15k-237 is composition. The results demonstrate the effectiveness of SpaceE to model the relation composition.

The results in Table 6 show that SpaceE gets the state-of-the-art performance on Hits@1, Hits@3, and Hits@10 metrics on YAGO3-10. The results are promising since YAGO3-10 is the largest dataset among the three datasets. It contains 123182 entities and more than one million fact triples. Most of the relations in YAGO3-10 are non-injective descriptive attributes of people such as wasBornIn and graduatedFrom. RotatE does not perform well on this dataset due to its limited ability for non-injective relation modeling. The high performances of SpaceE demonstrate its strong capability of non-injective relation modeling.

As shown in Table 5, SpaceE gets competitive results with RotatE on WN18RR. RotatE performs well on this dataset, although not well on FB15k-237 and YAGO3-10 datasets. We find two major reasons for this phenomenon. First, the non-injective relations which are difficult for RotatE are not prevalent in WN18RR. #hptr of relations in WN18RR is 2.9. Second, symmetry is prevalent in WN18RR. RotatE can take advantage of its bias - the composition of two symmetric relations is (incorrectly) symmetric [1].

One might wonder whether adding the augmented inverse relations and their embeddings can improve RotatE. We conduct the
### Table 4: Results on FB15k and WN18 datasets. Results with suffix [■] and [❤] are taken from Nickel et al. [28] and [14] respectively. Others are obtained from the original papers.

|           | FB15k       |           | WN18       |
|-----------|-------------|-----------|------------|
|           | MRR | H@1 | H@3 | H@10 | MRR | H@1 | H@3 | H@10 |
| DistMult  | 0.798 | -   | -   | 0.893 | 0.797 | -   | -   | 0.946 |
| ComplEx   | 0.692 | 0.599 | 0.759 | 0.840 | 0.941 | 0.936 | 0.945 | 0.947 |
| ConvE     | 0.657 | 0.558 | 0.723 | 0.831 | 0.943 | 0.935 | 0.946 | 0.956 |
| SE        | -     | -    | -    | 0.398 | -     | -    | -    | 0.805 |
| TransE[■] | 0.463 | 0.297 | 0.578 | 0.749 | 0.495 | 0.113 | 0.888 | 0.943 |
| TransH    | -     | -    | -    | 0.585 | -     | -    | -    | 0.867 |
| RotatE    | 0.797 | 0.746 | 0.830 | 0.884 | 0.949 | 0.944 | 0.952 | 0.959 |
| SpaceE    | 0.791 | 0.736 | 0.830 | 0.883 | 0.947 | 0.941 | 0.951 | 0.959 |

### Table 5: Results on FB15k-237 and WN18RR datasets. The results of TransE, DistMult, and ConvE are taken from Sun et al. [38], and others are obtained from the original papers. SE [7] and TransH [43] papers do not have results on the two datasets.

|           | FB15k-237       |           | WN18RR       |
|-----------|-----------------|-----------|--------------|
|           | MRR | H@1 | H@3 | H@10 | MRR | H@1 | H@3 | H@10 |
| DistMult  | 0.24 | 0.155 | 0.263 | 0.419 | 0.247 | 0.158 | 0.275 | 0.428 |
| ComplEx   | 0.247 | 0.158 | 0.275 | 0.428 | 0.44 | 0.41 | 0.46 | 0.51 |
| TuckER    | 0.358 |   | 0.394 | 0.544 | 0.470 | 0.443 | 0.482 | 0.526 |
| ConvE     | 0.325 | 0.237 | 0.356 | 0.501 | 0.325 | 0.237 | 0.356 | 0.501 |
| TransE    | 0.294 | -    | -    | 0.465 | 0.226 | -    | -    | 0.501 |
| RotatE    | 0.338 | 0.24  | 0.375 | 0.533 | 0.476 | 0.428 | 0.492 | 0.571 |
| BoxE      | 0.337 | -    | -    | 0.538 | 0.451 | -    | -    | 0.541 |
| SpaceE    | 0.351 | 0.253 | 0.389 | 0.544 | 0.473 | 0.423 | 0.496 | 0.570 |

### Table 6: Results on YAGO3-10 datasets. The results of DistMult is taken from Sun et al. [38]. Others are obtained from the origin papers.

|           | YAGO3-10       |
|-----------|----------------|
|           | MRR | H@1 | H@3 | H@10 |
| DistMult  | 0.340 | 0.240 | 0.380 | 0.540 |
| ComplEx   | 0.360 | 0.260 | 0.40 | 0.550 |
| TuckER    | 0.527 | 0.446 | 0.576 | 0.676 |
| ConvE     | 0.52 | 0.45 | 0.56 | 0.66 |
| RotatE    | 0.495 | 0.402 | 0.550 | 0.670 |
| BoxE      | 0.560 | -    | -    | 0.691 |
| MQuadE    | 0.536 | 0.449 | 0.592 | 0.689 |
| SpaceE    | 0.549 | **0.463** | **0.604** | **0.702** |

5.3 Results on Non-injective Relations

We compare our model with RotatE, the state-of-the-art translation distance based method on non-injective relations. Following previous works [38, 43], we study the ability to model the non-injective relations by categorizing relations into 1-to-1, 1-to-N, N-to-1, and N-to-N relations and report the performances of the four relation groups.

The FB15k-237 test set has 74 1-to-1 relation triples, 67 1-to-N relation triples, 1710 N-to-1 relation triples, and 18615 N-to-N relation triples. The Yago3-10 test set has 556 N-to-1 relation triples and 4444 N-to-N relation triples; it does not contain 1-to-1 and 1-to-N relation triples.

The results in Table 7 and Table 8 show that SpaceE consistently outperforms RotatE on N-N relations for both head and tail entity prediction, on 1-to-N relations for tail entity prediction, and on N-to-1 relations for head entity prediction.

The number of head entities attached to (t, r) (denoted by \( hptr \)) or the number of tail entities attached to (h, r) (denoted by \( tphr \)) can reflect the non-injective degree of the relation in a fact triple. The Yago3-10 dataset has the largest average number of heads per tail and relations (\( #hptr \)) among the five datasets, so we use it to investigate the relationship between the head prediction performance and \( hptr \).

We compare the head prediction performances of RotatE and SpaceE on test triples with different \( hptr \). The test triples are categorized into five groups by their \( hptr \): \([0, 10]\), \([11, 50]\), \([51, 100]\), \([101, 1000]\), and \([1001, 10000]\). The average number of \( hptr \) of the triples in the five groups is 4, 28, 74, 273, and 46678. The number of test triples in the five categories is 987, 913, 692, 2016, and 374.

From the results in Table 9, we observe that: 1) SpaceE consistently outperforms RotatE in terms of all evaluation metrics on the five \( hptr \) triple categories; 2) when \( hptr \leq 10 \), SpaceE beats RotatE.
Table 7: Results of RotatE and SpaceE on different relation types of the FB15k-237 dataset. H denotes head prediction performances, T denotes tail prediction performances.

| Metric | Model  | 1-1 | 1-N | N-1 | N-N |
|--------|--------|-----|-----|-----|-----|
|        |        | H   | T   | H   | T   | H   | T   |
| MRR    | RotatE | 1   | 1   | 0.885 | 0.168 | 0.095 | 0.847 | 0.243 | 0.389 |
|        | SpaceE | 1   | 1   | 0.657 | 0.267 | 0.152 | 0.831 | 0.259 | 0.41  |
| H@10   | RotatE | 1   | 1   | 0.985 | 0.239 | 0.159 | 0.911 | 0.441 | 0.610 |
|        | SpaceE | 1   | 1   | 0.985 | 0.582 | 0.228 | 0.905 | 0.455 | 0.624 |

Table 8: Head prediction and tail prediction results of RotatE and SpaceE on different relation types of the Yago3-10 dataset. H and T denote head prediction and tail prediction, respectively.

| Metric | Model  | N-to-1 | N-to-N |
|--------|--------|--------|--------|
|        |        | H     | T     | H     | T     |
| MRR    | RotatE | 0.01  | 0.66  | 0.38  | 0.64  |
|        | SpaceE | 0.02  | 0.65  | 0.45  | 0.69  |
| H@10   | RotatE | 0.04  | 0.79  | 0.61  | 0.79  |
|        | SpaceE | 0.04  | 0.80  | 0.65  | 0.81  |

Table 9: The head entity prediction performances of RotatE and SpaceE on triples with different hptr in the YAGO3-10 dataset.

| hptr group | 1     | 2     | 3     | 4     | 5     |
|------------|-------|-------|-------|-------|-------|
|            | MRR   |       |       |       |       |
|            | RotatE | 0.35  | 0.45  | 0.42  | 0.32  | 2e-3  |
|            | SpaceE | 0.37  | 0.52  | 0.53  | 0.41  | 3e-3  |
|            | H@1   |       |       |       |       |
|            | RotatE | 0.27  | 0.34  | 0.28  | 0.18  | 0     |
|            | SpaceE | 0.30  | 0.42  | 0.41  | 0.28  | 0     |
|            | H@3   |       |       |       |       |
|            | RotatE | 0.38  | 0.53  | 0.52  | 0.37  | 0     |
|            | SpaceE | 0.40  | 0.59  | 0.60  | 0.47  | 0     |
|            | H@10  |       |       |       |       |
|            | RotatE | 0.48  | 0.64  | 0.69  | 0.60  | 3e-3  |
|            | SpaceE | 0.49  | 0.67  | 0.73  | 0.64  | 0.01  |

with more than 0.01 absolute improvement; when 100 ≤ hptr ≤ 1000, the improvement of SpaceE over RotatE is more substantial, with about 0.10 absolute improvement on MRR and Hits@1, 3.

5.4 Case Studies on Relation Patterns

The relation matrix representation of SpaceE provides insights into the property of the relation.

Symmetry/skew-symmetry. We plot the contours of $|\hat{R}_3|$, $|\hat{R}_2|$ for a relation $r$. Figure 1a and Figure 1b show that for symmetric relations similar_to and verb_group in the WN18 dataset, the matrix $|\hat{R}_3|$ is similar to the identity matrix. Figure 1c and Figure 1d show that for skew-symmetric relations hypernym and hyponym, the matrix looks different from the identity matrix.

Inversion. We plot the contours of $|\hat{R}_1 \hat{R}_3|$ for two relations $r_1$ and $r_2$ that are the inverses of each other. As shown in Figure 1e and Figure 1f, $|\hat{R}_1 \hat{R}_3|$ approximates the identity matrix for inversion relation pairs hypernym ⊗ hyponym and has_part ⊗ part_of in the WN18 dataset. It confirms that SpaceE is able to model the inversion of the relation by the inversion of the relation matrix.

Composition. For three relations for2, winner, for1 in FB15k-237 dataset, for2 = winner ⊗ for1, we denote their relation matrices as $R_3$, $R_1$, $R_2$. Let $\hat{R}_2$ be the augmented inverse relation of $\hat{R}_2$ and $\hat{R}_1$ be its relation matrix. We plot the contours of $|\hat{R}_1 \hat{R}_3|$ and $|\hat{R}_1 \hat{R}_2|$ in Figure 1g and Figure 1h, respectively. It shows that the matrices $|\hat{R}_1 \hat{R}_3|$ and $|\hat{R}_1 \hat{R}_2|$ look similar to the identity matrix. The values in the diagonal positions are larger than the values in other positions. Thus, $R_3 = R_1 R_2$.

6 CONCLUSION

The general philosophy of representation learning is to automatically discover the representations of input data in order to make appropriate decisions. Two fundamental problems in representation learning are (i) the form of representations and (ii) the decision function. The mathematical properties of the representation form and the decision function determine the learning ability of the learning machine.

In this paper, we study the ability of representation learning algorithms in knowledge graph reasoning. We show that the relationships in knowledge graphs vary in their logical properties, including injective vs. non-injective, Abelian vs. Non-Abelian, etc. Furthermore, the reasoning procedure in the knowledge graph builds logical connections between relations, such as inversion and composition. These logical properties and connections exert mathematical constraints on the representation form and the decision function. Improper design of the representation form and the decision function may fail in implementing those logical properties and connections. We demonstrate that the theoretical failures indeed happened in existing methods.

As the solution to implementing all these logical properties and connections, we propose a translation distance-based knowledge graph embedding method called SpaceE using the idea of modeling relations as linear transformations in the entity space. We theoretically demonstrate the ability of SpaceE to model various relation properties, including injective, non-injective, symmetry, skew-symmetry, inversion, Abelian composition, and non-Abelian composition. Qualitative case studies show that the property of learned relation matrices can reflect the symmetry, skew-symmetry, inversion, and composition of relations. Experiments on five benchmark datasets show that our model obtains competitive results on
Although our method in this paper is proposed and tested only in knowledge graph reasoning, our design can potentially be applied to other fields that involve complex logical properties and connections, such as many problems in causal discovery. It is a long road to find a general representation learning solution for all kinds of logical relations. It is admitted that we have only made a small step forward down the road.

REFERENCES

[1] Ralph Abboud, Ismael Ilkay Ceylan, Thomas Lukasiewicz, and Tommaso Salvadori. 2020. BoxE: A Box Embedding Model For Knowledge Base Completion. In Advances in Neural Information Processing Systems (NeurIPS) virtual.

[2] Ivana Balazevic, Carl Allen, and Timothy M. Hospedales. 2019. TuckER: Tensor Factorization for Knowledge Graph Completion. In Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP). Hong Kong, China, 5184–5193.

[3] Michele Banko, Michael J. Cafarella, Stephen Soderland, Matthew Broadhead, and Oren Etzioni. 2007. Open Information Extraction from the Web. In Proceedings of the 20th International Joint Conference on Artificial Intelligence (IJCAI). Hyderabad, India, 2670–2676.

[4] Nitin Bansal, Xiaohan Chen, and Zhangyang Wang. 2018. Can We Gain More from Orthogonality Regularizations in Training Deep Networks? In Advances in Neural Information Processing Systems (NeurIPS). Montréal, Canada, 4266–4276.

[5] Kurt D. Bollacker, Colin Evans, Praveen K. Paritosh, Tim Sturge, and Jamie Taylor. 2008. Freebase: a collaboratively created graph database for structuring human knowledge. In Proceedings of the ACM SIGMOD International Conference on Management of Data (SIGMOD). Vancouver, Canada, 1247–1250.

[6] Antoine Bordes, Nicolas Usunier, Alberto Garcia-Duran, Jason Weston, and Oksana Yakhnenko. 2013. Translating Embeddings for Modeling Multi-relational Data. In Advances in Neural Information Processing Systems (NIPS). Lake Tahoe, NV, 2787–2795.

[7] Antoine Bordes, Jason Weston, Ronan Collobert, and Yoshua Bengio. 2011. Learning Structured Embeddings of Knowledge Bases. In Proceedings of the Twenty-Fifth AAAI Conference on Artificial Intelligence (AAAI). San Francisco, CA.

[8] Xiaojun Chen, Shengbin Jia, and Yang Xiang. 2020. A review: Knowledge reasoning over knowledge graph. Expert Syst. Appl. 141 (2020).

[9] Zeyu Dai, Hengliang Fei, and Ping Li. 2019. Coreference Aware Representation Learning for Named Entity Recognition. In Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence (IJCAI). Macao, China, 4946–4953.

[10] Tim Dettmers, Pasquale Minervini, Pontus Stenetorp, and Sebastian Riedel. 2018. Convolutional 2D Knowledge Graph Embeddings. In Proceedings of the Thirty-Second AAAI Conference on Artificial Intelligence (AAAI). New Orleans, LA, 1811–1818.

[11] Takanori Ebisu and Ryutaro Ishie. 2018. TorusE: Knowledge Graph Embedding on a Lie Group. In Proceedings of the Thirty-Second AAAI Conference on Artificial Intelligence (AAAI). New Orleans, LA, 1819–1826.

[12] Swapnil Gupta, Sreyash Kenkre, and Partha P. Talukdar. 2019. CalRE: Open Knowledge Graph Embeddings. In Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP). Hong Kong, China, 378–388.

[13] Xiao Huang, Jingyuan Zhang, Dingcheng Li, and Ping Li. 2019. Knowledge Graph Embedding Based Question Answering. In Proceedings of the Twelfth ACM International Conference on Web Search and Data Mining (WSDM). Melbourne, Australia, 105–113.

[14] Rudolf Kadlec, Ondrej Bajgar, and Jan Kleindienst. 2017. Knowledge Base Completion: Baselines Strike Back. In Proceedings of the 2nd Workshop on Representation Learning for NLP (RepNLP@ACL). Vancouver, Canada, 69–74.

[15] Seyed Mehran Kazemi and David Poole. 2018. Simple Embedding for Link Prediction in Knowledge Graphs. In Advances in Neural Information Processing Systems (NeurIPS). Montréal, Canada, 4289–4300.

[16] Petar Mullenik P. Kingsma and Jimmy Ba. 2015. Adam: A Method for Stochastic Optimization. In Proceedings of the 3rd International Conference on Learning Representations (ICLR). San Diego, CA.

[17] Timothée Lacroix, Nicolas Usunier, and Guillaume Obozinski. 2018. Canonical Tensor Decomposition for Knowledge Base Completion. In Proceedings of the 35th International Conference on Machine Learning (ICML). Stockholmsmässan, Stockholm, Sweden, 2869–2878.

[18] Ni Lao and William W. Cohen. 2010. Relational retrieval using a combination of path-constrained random walks. Mach. Learn. 81, 1 (2010), 53–67.

[19] Ni Lao, Tom M. Mitchell, and William W. Cohen. 2011. Random Walk Inference and Learning in A Large Scale Knowledge Base. In Proceedings of the 2011 Conference on Empirical Methods in Natural Language Processing (EMNLP). Edinburgh,
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abstract = {Translation distance based knowledge graph embedding (KGE) methods, such as TransE and RotatE, model the relation in knowledge graphs as translation or rotation in the vector space. Both translation and rotation are injective; that is, the translation or rotation of different vectors results in different results. In knowledge graphs, different entities may have a relation with the same entity; for example, many actors starred in one movie. Such a non-injective relation pattern cannot be well modeled by the translation or rotation operations in existing translation distance based KGE methods. To tackle the challenge, we propose a translation distance-based KGE method called SpaceE to model relations as linear transformations. The proposed SpaceE embeds both entities and relations in knowledge graphs as matrices and SpaceE naturally models non-injective relations with singular linear transformations. We theoretically demonstrate that SpaceE is a fully expressive model with the ability to infer multiple desired relation patterns, including symmetry, skew-symmetry, inversion, Abelian composition, and non-Abelian composition. Experimental results on link prediction datasets illustrate that SpaceE substantially outperforms many previous translation distance based knowledge graph embedding methods, especially on datasets with many non-injective relations. The code is available based on the PaddlePaddle deep learning platform https://www.paddlepaddle.org.cn/},
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