RETHINKING IDENTITY IN KNOWLEDGE GRAPH EMBEDDING

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ABSTRACT

Knowledge Graph Embedding (KGE) is a common method to complete real-world Knowledge Graphs (KGs) by learning the embeddings of entities and relations. Beyond specific KGE models, previous work proposes a general framework based on group. A group has a special element **identity** that uniquely corresponds to the relation *identity* in KGs, which implies that *identity* should theoretically have a unique representation. However, we find that this uniqueness cannot be modeled by bilinear based models, revealing the crack between the framework and models. To this end, we study the conditions required for modeling such uniqueness and propose a modification model named Unit Ball Bilinear Model (UniBi). Beyond the theoretical advantage, UniBi is more robust and interpretable. Experiments demonstrate that UniBi models the uniqueness without the cost of performance and verify its a robustness and interpretability.

1 INTRODUCTION

Knowledge Graphs (KGs) store human knowledge in the form of triple (h, r, t), which represents a relation r between a head entity h and a tail entity t Ji et al. (2021). KGs benefit a lots of downstream tasks and applications, e.g., recommender system Zhang et al. (2016), dialogue system He et al. (2017) and question answering Mohammed et al. (2018). Since actual KGs are usually incomplete, researchers are interested in predicting missing links to complete them. As a common solution, Knowledge Graph Embedding (KGE) completes KGs by learning low-dimensional representations of entities and relations.

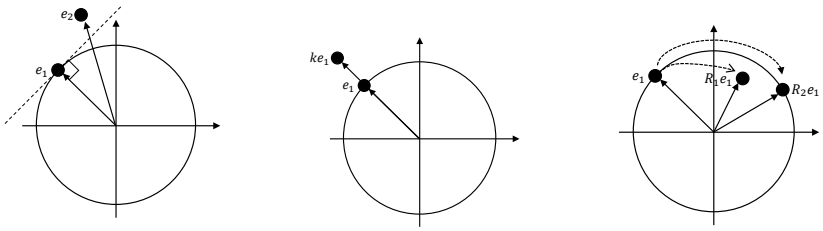
Beyond the great advances in specific KGE models Trouillon et al. (2016); Hitchcock (1927); Chami et al. (2020); Liu et al. (2017); Nickel et al. (2011); Bordes et al. (2013), Several works also attempt to unify these models with general frameworks, such as promising ones based on groupYang et al. (2020); Xu & Li (2019); Ebisu & Ichise (2018). Since each group has a special element **identity** it requires that the *identity* relation in the corresponding KG should have a unique representation theoretically. However, we find that such uniqueness cannot be modeled by bilinear based models, which reveals the crack between the framework and models.

More specifically, a model with score function $s(h, r, t)$ can model the uniqueness of *identity* means that $\forall h \neq t, s(h, r, h) > s(h, r, t)$ holds if and only if r is *identity*. In addition, the score function $s(\cdot)$ of bilinear based model is $\mathbf{h}^\top \mathbf{R}\mathbf{t}$, where $\mathbf{h}, \mathbf{R}, \mathbf{t}$ are the representations for h, r, and t.

In terms of such uniqueness, bilinear based models have two flaws. In Fig. 1(a), we notice that $\mathbf{e}_1^\top \mathbf{I}\mathbf{e}_1 < \mathbf{e}_1^\top \mathbf{I}\mathbf{e}_2$, which means that the relation matrices per se do not model $identity$ perfectly. Furthermore, even if it is a matrix, e.g. $\mathbf{I}$, does. Its scaled one $k\mathbf{I}$ where $k > 0, k \neq 1$ can also model the *identity* and thus breaks its uniqueness, as demonstrated in Fig. 1(b).

To this end, we replace bilinear based models by a modified one proven to satisfy such property. The proposed model is achieved by normalizing the vectors of the entities and restricting the spectral radius to 1 for the metrics of the relations. Since the model captures entities in a unit ball as shown in Fig. 1(c), we name it Unit Ball Bilinear Model (UniBi).

Beyond the theoretical advantage, UniBi is more robust and interpretable. On the one hand, UniBi inherently subsumes DURA, the best regularization term for bilinear based models Zhang et al. (2020a), in the perspective of Lagrangian functions. On the other hand, UniBi interprets the norms



(a) (b) (c)

Figure 1: The flaws of bilinear based models and our solution dealing with modeling the uniqueness of *identity*. (a) Identity matrix fails to model *identity*. (b) Scaled identity matrix could also model *identity*. (c) An illustration of UniBi. All entities are embedded in the unit sphere and stay in the unit ball after relation specific transformations.

of entities as their certainty and captures the character that the certainty will not increase under any relation.

Experiments verify that UniBi models *identity* uniquely without the cost of performance. Furthermore, UniBi demonstrates its robustness and interpretability. Therefore, UniBi fills the gap between the general framework and the specific models in terms of *identity* and paves the way for further studies of both.

2 PRELIMINARIES

2.1 BACKGROUND

A Knowledge Graph $\mathcal{K}$ is a set that contains the facts about sets of entities $\mathcal{E}$ and relations $\mathcal{R}$. Each fact is stored by a triple $(e_i, r_j, e_k) \in \mathcal{E} \times \mathcal{R} \times \mathcal{E}$ where e_i and r_j denote the i -th entity and the j -th relation, respectively.

KGE aims to predict the missing links in $\mathcal{K}$ by learning embeddings for each entity and relation via a score function $s : \mathcal{E} \times \mathcal{R} \times \mathcal{E} \rightarrow \mathbb{R}$. To verify the performance of a KGE method, $\mathcal{K}$ is first divided into $\mathcal{K}_{train}$ and $\mathcal{K}_{test}$. Then, the method is trained on $\mathcal{K}_{train}$ to learn the embeddings $\mathbf{e}$ and $\mathbf{r}$ for each entity $e \in \mathcal{E}$ and relation $r \in \mathcal{R}$. Finally, for each query $(e_i, h_j, ?)$ from $\mathcal{K}_{test}$ and the candidate entity $e_k \in \mathcal{E}$, the model is expected to give it a higher rank if $(e_i, h_j, e_k) \in \mathcal{K}$ and a lower rank if $(e_i, h_j, e_k) \notin \mathcal{K}$.

Although in addition to the above tail prediction, models are also required to test on head prediction conversely, previous study Lacroix et al. (2018) has shown that this task can be transformed to tail prediction by introducing reciprocal relations.

To avoid confusion, we use bold to represent the element **identity** while italics to represent *identity* and other relations. Furthermore, we give the definitions of monoid, group, and *identity* discussed in the latter.

Definition 1 (Jacobson (2012))**.** *A monoid is a triple $(M, p, 1$ in which M is a non-vacuous set, p is an associative binary composition (or product) in M, and 1 is an element of M such that $p(1, a) = a = p(a, 1)$ for all $a \in M$*

Definition 2 (Jacobson (2012))**.** *A group G (or (G,p,1)) is a monoid all of whose elements are invertible.*

Definition 3. *A KGE model can uniquely model identity means there is only one $r \in \mathcal{R}$ and has $s(h, r, h) > s(h, r, t)$, $\forall h, t \in \mathcal{E}, h \neq t$. And the ideal representation of such relation is unique.*

2.2 OTHER NOTATIONS

We utilize $\hat{\mathbb{E}}$ and $\hat{\mathbb{R}}$ to denote the set of all possible representations of entities and relations. And we use $\mathbf{e} \in \hat{\mathbb{E}}$ and $\mathbf{R} \in \hat{\mathbb{R}}$ to denote the embedding vector of the entity e and the transformation matrix

specific to the relation $\mathbf{R}$. Furthermore, we use $\|\cdot\|$ to denote the L2 norm of the vectors, $\|\cdot\|_F$ and $\rho(\cdot)$ to represent the Frobenius norm and the spectral radius of a matrix.

In this paper, we focus on n-dimensional real space $\mathbb{R}^n$, which means $\hat{\mathbb{E}} \subset \mathbb{R}^n$ and $\hat{\mathbb{R}} \subset \mathbb{R}^{n\times n}$. Furthermore, for other real vector spaces whose vectors are complex $\mathbb{C}^n$ or hypercomplex space $\mathbb{H}^n$, they are also being considered since they can be transformed to their isomorphism on $\mathbb{R}^{2n}$ or $\mathbb{R}^{4n}$.

3 Related Work

Previous work of KGE can be roughly divided into the following three categories: distance, bilinear and others.

Distance based models choose Euclidean distance for their score functions. TransE Bordes et al. (2013) inspired by Word2Vec Mikolov et al. (2013) in Natural Language Processing proposes the first distance based model, which uses translation as the linear transformation $s(h,r,t) = -\|\mathbf{h}+\mathbf{r}-\mathbf{t}\|$. TransH Lin et al. (2015) and TransR Lin et al. (2015) find that TransE difficult to handle complex relations and thus apply linear projections before translation. Apart from translation, RotatE Sun et al. (2019) first introduces rotation as the transformation. RotE Chami et al. (2020) further combines translation and rotation. Some works also introduce hyperbolic spaces Balazevic et al. (2019b); Chami et al. (2020); Wang et al. (2021). Apparently, distance based models are born to uniquely model *identity*, since the distance between a vector and itself is 0 [1].

In contrast, bilinear based models have score functions in the bilinear form $s(h,r,t) = \mathbf{h}^\top\mathbf{R}\mathbf{t}$. RESCAL Nickel et al. (2011) is the first bilinear based model whose relation matrices are unconstrained. Although RESCAL is expressive, it contains too many parameters and tends to overfitting. DistMult Yang et al. (2015) simplifies these matrices into diagonal ones. ComplEx Trouillon et al. (2016) further introduces complex values to model the skew-symmetry pattern. Analogy Liu et al. (2017) uses block-diagonal to model the analogical pattern and subsumes DistMult, ComplEx, and HolE Nickel et al. (2016). Moreover, QuatE Zhang et al. (2019) extends complex values to quaternion and GeomE Xu et al. (2020) utilizes geometric algebra to subsume all these models. However, these studies have not noticed that bilinear based models fail to uniquely model *identity*.

Corresponding to *identity*, **identity** is a special element in the group. The group is first mentioned by Dihedral Xu & Li (2019) and HolE Nickel et al. (2016). Based on the group, NagE Yang et al. (2020) proposes a general framework to incorporate previous methods. Although they believe that the matrix representation for *identity* is $\mathbf{I}$, they do not bother to explore that *identity* may not be uniquely modeled by specific models.

In addition, other works using black-box networks Dettmers et al. (2018); Nguyen et al. (2018); Yao et al. (2019); Schlichtkrull et al. (2018); Zhang et al. (2020b) or additional information An et al. (2018); Ren et al. (2016) are beyond the scope of this paper.

4 Method

In this section, we first discuss the relationship between the **identity** element in groups and the *identity* relation in KGs, and give the condition for modeling *identity* uniquely in Section 4.1. We then propose a model named UniBi that satisfies it in Section 4.2 and an efficient modeling for UniBi in Section 4.3. In addition, we also discuss its properties in Section 4.4.

4.1 Identity and *Identity*

In previous work, a framework based on group has been proposed Yang et al. (2020). It states that all relations should be embedded as elements of a group. Groups have a special element **identity**, which corresponds to the *identity* relation in KGs. This correspondence implies that the *identity* relation should have a unique embedding theoretically.

Although this seems easy to satisfy, we find that in fact bilinear based models fails to model this uniqueness. We demonstrate two cases in which bilinear based models violate it. In Fig. 1(a), we

[1] We also prove this more rigorously in Appendix B

notice that $\mathbf{e}_1^\top \mathbf{I} \mathbf{e}_1 < \mathbf{e}_1^\top \mathbf{I} \mathbf{e}_2$, which means that the matrix of a relation per se is not guaranteed for modeling *identity*. As demonstrated in Fig. 1(b), even if it can be modeled by a matrix, e.g. $\mathbf{I}$. Its scaled result $k\mathbf{I}$ where $k > 0, k \neq 1$ can also model the *identity*, which contradicts the quantification of uniqueness. Therefore, to investigate how to modify bilinear based models to model this uniqueness, we give a formal definition based on definition 3 as following.

Definition 4. *A bilinear model can uniquely model identity means:*

$$\exists!\, \mathbf{R} \in \hat{\mathbb{R}}, \forall \mathbf{h}, \mathbf{t} \in \hat{\mathbb{E}}, \mathbf{h} \neq \mathbf{t},\ \mathbf{h}^\top \mathbf{R} \mathbf{h} > \mathbf{h}^\top \mathbf{R} \mathbf{t}, \tag{1}$$

where $\exists!$ *is the uniqueness quantification.*

4.2 Unit Ball Bilinear Model

From the above examples, it is clear that both embeddings of entities and relations needed to be constrained. Specifically, the former is supposed to be located in a sphere while the latter needs to contain $\mathbf{I}$ while exclude $k\mathbf{I}$ for $k > 0, k \neq 1$.

Following the above intuition, we propose Unit Ball Bilinear Model (UniBi) by adding constraints. UniBi sets $\hat{\mathbb{E}} = \{\mathbf{e} \,|\, \|\mathbf{e}\| = 1, \mathbf{e} \in \mathbb{R}^n\}$ and $\hat{\mathbb{R}} = \{\mathbf{R} \,|\, \rho(\mathbf{R}) = 1, \mathbf{R} \in \mathbb{R}^{n \times n}\}$ and has a score function as[2]:

$$s(h, r, t) = \mathbf{h}^\top \mathbf{R} \mathbf{t},\ \|\mathbf{h}\|, \|\mathbf{t}\| = 1, \rho(\mathbf{R}) = 1. \tag{2}$$

We then have the following theorem.

Theorem 1. *UniBi is capable to uniquely model identity in terms of definition 4.*

Proof. Please refer to the Appendix A.2 □

4.3 Efficient Modeling

4.3.1 Efficient Modeling for Spectral Radius

Although the proposed model is proven to uniquely model *identity*, it still has a practical disadvantage since it is difficult to directly represent all matrices whose spectral raidus are 1. In addition, it is time-consuming to calculate the spectral radius $\rho(\cdot)$ via singular values decomposition (SVD).

To avoid decomposing recurrently, we divide a relation matrix into three parts $\mathbf{R} = \mathbf{R}_h \mathbf{\Sigma} \mathbf{R}_t$ where $\mathbf{R}_h, \mathbf{R}_t$ are orthogonal matrices and $\mathbf{\Sigma} = \text{Diag}[\sigma_1, \ldots, \sigma_n]$ is a positive semidefinite diagonal matrix. And we maintain the independence of these three components during training. Therefore, it becomes simple to obtain matrices whose spectral radius is 1, that is, $\frac{\mathbf{R}_h \mathbf{\Sigma} \mathbf{R}_t}{\sigma_{max}}$. And we transform the score function equation 2 into the following form.

$$s(h, r, t) = \frac{\mathbf{h}^\top \mathbf{R}_h \mathbf{\Sigma} \mathbf{R}_t \mathbf{t}}{\sigma_{max} \|\mathbf{h}\| \|\mathbf{t}\|}, \tag{3}$$

where σ_{max} is the maximum among σ_i.

4.3.2 Efficient Modeling for Orthogonal Matrix

In addition, we find that the calculation of the orthogonal matrix is still time-consuming Tang et al. (2020). To this end, we only consider the diagonal orthogonal block matrix, where each block is a low-dimensional orthogonal matrix. Specifically, we use k-dimensional rotation matrices to build $\mathbf{R}_h$ and $\mathbf{R}_t$. Taking $\mathbf{R}_h$ as an example $\mathbf{R}_h = \text{Diag}[\mathbf{SO}(k)_1, \ldots, \mathbf{SO}(k)_{\frac{n}{k}}]$, where $\mathbf{SO}(k)_i$ denotes the i-th special orthogonal matrix, that is, the rotation matrix.

The rotation matrix only represents the orthogonal matrices whose determinant are 1 and does not represent the ones whose determinant are -1. To this end, we introduce two diagonal sign matrices of n-th order $\mathbf{S}_h, \mathbf{S}_t \in \mathbb{S}$ where

$$\mathbb{S} = \{\mathbf{S} \mid \mathbf{S}_{ij} = \begin{cases} \pm 1, & if\ i = j, \\ 0, & if\ i \neq j. \end{cases}\}. \tag{4}$$

[2]We present in more detail the similarities and differences between our constraints and those of our predecessors in the Appendix C.

Thus, we could rewrite the score function equation 3 to

$$s(h,r,t) = \frac{\mathbf{h}^\top \mathbf{R}_h \mathbf{S}_h \mathbf{\Sigma} \mathbf{S}_t \mathbf{R}_t \mathbf{t}}{\sigma_{max} \|\mathbf{h}\| \|\mathbf{t}\|}. \tag{5}$$

However, the sign matrix $\mathbf{S}_h$ and $\mathbf{S}_t$ are discrete. To address this problem, we notice that $\mathbf{S}_h$, $\mathbf{\Sigma}$, $\mathbf{S}_t$ can be merged into a matrix $\mathbf{\Xi}$ that

$$\mathbf{\Xi}_{ij} = \begin{cases} s_i s_j \sigma_i, & if\ i = j, \\ 0 & if\ i \neq j. \end{cases} \tag{6}$$

where $s_i = (\mathbf{S}_h)_{ii}$, $s_j = (\mathbf{S}_t)_{jj}$, $i, j = 1, \ldots, n$ and $\mathbf{\Xi} = \text{Diag}[\xi_1, \ldots, \xi_n]$. Thus, we incorporate the discrete matrices $\mathbf{S}_h, \mathbf{S}_t$ into the continuous matrix $\mathbf{\Xi}$.

$$s(h,r,t) = \frac{\mathbf{h}^\top \mathbf{R}_h \mathbf{\Xi} \mathbf{R}_t \mathbf{t}}{|\xi_{max}| \|\mathbf{h}\| \|\mathbf{t}\|}, \tag{7}$$

where $|\xi_{max}|$ is the maximum among $|\xi_i|$.

4.4 Further analyze on constraints of UniBi

In addition to modeling *identity* uniquely, the constraints of UniBi enhance the robustness and the interpretability of bilinear based models.

4.4.1 Robustness from Inherent Regularization

We first discover the necessary constraints of UniBi and then deduce its corresponding Lagrangian function.

Theorem 2. *UniBi has a set of necessary constraints that* $\|\mathbf{e}\| = 1$, $\|\mathbf{R}\mathbf{e}\| \leq 1$ *and* $\|\mathbf{R}^\top \mathbf{e}\| \leq 1$.

Proof. Please refer to the Appendix A.3. □

If we ignore the other implicit constraints, the optimization of UniBi can be rewritten in the form of a constrained optimization problem.

$$\begin{aligned} \min_{\mathbf{h},\mathbf{r},\mathbf{t}} & \sum_{(h_i,r_j,t_k)\in\mathcal{K}} f(h_i, r_j, t_k) \\ s.t.\ & \|\mathbf{h}_i\|^2 = 1, \|\mathbf{t}_k\|^2 = 1 \\ & \|\mathbf{R}_j^\top \mathbf{h}_i\|^2 \leq 1, \|\mathbf{R}_j \mathbf{t}_k\|^2 \leq 1, \end{aligned} \tag{8}$$

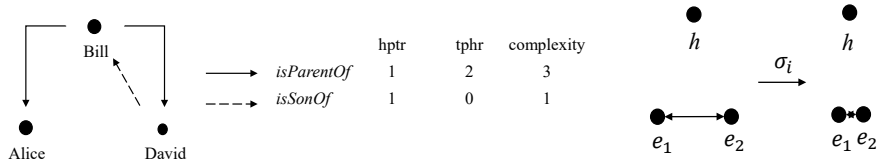
where $f(h,r,t)$ is loss function. Furthermore, Eq. equation 8 corresponds to a Lagrangian function.

$$\begin{aligned} \min_{\mathbf{h},\mathbf{r},\mathbf{t},\lambda,\mu} & \sum_{(h_i,r_j,t_k)\in\mathcal{K}} f(h_i, r_j, t_k) + \lambda_i^h(\|\mathbf{h}_i\|^2 - 1) + \lambda_k^t(\|\mathbf{t}_k\|^2 - 1) \\ & + \mu_j^h(\|\mathbf{R}_j^\top \mathbf{h}_i\|^2 - 1) + \mu_j^t(\|\mathbf{R}_j \mathbf{t}_k\|^2 - 1) \\ s.t.\ & \mu_j^h, \mu_j^t \geq 0. \end{aligned} \tag{9}$$

We notice that if we set factors $\lambda_i^h = \lambda_k^t = \lambda\lambda_1$ and $\mu_j^h = \mu_j^t = \lambda\lambda_2$ where $\lambda, \lambda_1, \lambda_2 > 0$, we achieve the following expression from Eq. equation 9 by discarding constant terms[3].

$$\min_{\mathbf{h},\mathbf{r},\mathbf{t}} \sum_{(h_i,r_j,t_k)\in\mathcal{K}} f(h_i, r_j, t_k) + \lambda \left[\lambda_1(\|\mathbf{h}_i\|^2 + \|\mathbf{t}_k\|^2) + \lambda_2(\|\mathbf{R}_j^\top \mathbf{h}_i\|^2 + \|\mathbf{R}_j \mathbf{t}_k\|^2)\right], \tag{10}$$

which is equivalent to the optimization of a unconstrained model under DURA Zhang et al. (2020a), the best regularization term for bilinear based model before. Therefore, we find that UniBi contains DURA as an inherent regularization, which implies that UniBi is more robust than the unconstrained models.



(a) (b)

Figure 2: Complexity and aggregation. (a) A toy example to show how to calculate complexity. (2) the aggregation corresponds to the singular values less than 1.

4.4.2 INTERPRETABILITY FROM SINGULAR VALUE

In addition to robustness, our restriction on relations helps us to understand complex relations. Complex relations are defined by whither hptr (*h*ead *p*er *t*ail of a *r*elation) and tphr (*t*ail *p*er *h*ead of a *r*elation) is higher than a special threshold 1.5 Wang et al. (2014). Therefore, all relations are divided into 4 types, i.e. 1-1, 1-N, N-1 and N-N. However, we think this division is too coarse-grained and suggest that we should utilize a fine-grained continuing matrix complexity instead. To better demonstrate this idea, we gave an example in Fig. 2(a) and definition as follows.

Definition 5. *The complexity of a relation is the sum of its hptr and tphr.*

By adopting the idea that complex relations are handled by aggregating entities through projection Wang et al. (2014); Lin et al. (2015). As demonstrated in Fig. 2(b), the entities e_1 and e_2 are pulled very close and makes it easier for the model to give them the same score.

We find that such an aggregation is achieved by the singular values that are smaller than 1. Since for any relation matrix $\mathbf{R} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$, both $\mathbf{U}$ and $\mathbf{V}$ are isometry, and only the scaling matrix $\mathbf{\Sigma}$ can aggregate the entities. Correspondingly, such aggregation are perfectly modeled by the restriction of spectral radius, because it enforce the singular values less than or equal to 1[4]. In other words, the singular value σ_i of i-th dimension determines the degree of aggregation of that dimension as demonstrated in Fig. 2(b). Therefore, we could use singular values represent complexity of relations, which increases the interpretability of UniBi.

It is worth mentioning that this interpretabity can be transferred to other bilinear based models if they normalize the spectral radius of their relation matrix as UniBi do.

5 EXPERIMENT

In this section, we give the experiment settings in Section 5.1. We verify that UniBi is capable to uniquely model *identity*, while previous bilinear based models is not in Section 5.2. UniBi is comparable to previous SOTA bilinear models in the link prediction task, as shown in Section 5.3. In addition, we demonstrate the robustness of UniBi in Section 5.4 and correlation to complexity in Section 5.5.

Table 1: Statistics of the benchmark datasets.

Dataset	$\lvert\mathcal{E}\rvert$	$\lvert\mathcal{R}\rvert$	Training	Validation	Test
WN18RR	40,943	11	86,835	3,034	3,134
FB15k-237	14,541	237	272,115	17,535	20,466
YAGO3-10-DR	122,873	36	732,556	3,390	3,359

[3]This is not our final optimization function, it is only used to analyze the robustness.

[4]We will discuss this characteristic in more depth from the perspective of group in Appendix D.

5.1 EXPERIMENT SETTINGS

Dataset We evaluate models on three commonly used benchmarks, i.e. WN18RR Dettmers et al. (2018), FB15k-237 Toutanova & Chen (2015) and YAGO3-10-DR Akrami et al. (2020). They are proposed by removing the reciprocal triples that cause data leakage in WN18, FB15K and YAGO3-10 respectively. Their statistics are listed in Tbl. 5.

Evaluation metrics We use Mean Reciprocal Rank (MRR) and Hits@k (k = 1, 3, 10) as the evaluation metrics. MRR is the average inverse rank of the correct entities that are insensitive to outliers. Hits@k denotes the proportion of correct entities ranked above k.

Baselines Here we consider two specific versions of UniBi: UniBi-O(2), UniBi-O(3), which use rotation matrices in 2 and 3 dimensions to construct the orthogonal matrix. To be specific, we use the unit complex value and the unit quaternion to model the 2D and 3D rotations using the 2×2 and 4×4 matrices, respectively. For more details, see the Appendix E.1.

UniBi is compared with these bilinear models: RESCAL Nickel et al. (2011), CP Hitchcock (1927), ComplEx Trouillon et al. (2016), and QuatE Zhang et al. (2019). In addition, it also compared to other models: RotatE Sun et al. (2019), MurE Balazevic et al. (2019b) and RotE Chami et al. (2020), Turcker Balazevic et al. (2019a) and ConvE Dettmers et al. (2018).

Optimization We adopt the reciprocal setting Lacroix et al. (2018), which creates a reciprocal relation r' for each r and a new triple (e_k, r'_j, e_i) for each $(e_i, r_j, e_k) \in \mathcal{K}$. Instead of using Cross Entropy directly Lacroix et al. (2018); Zhang et al. (2020a; 2019), we add an extra scalar $\gamma > 0$ before softmax function. Since UniBi is bounded, it brings an upper bound to loss that makes the model difficult to optimize as discussed in Wang et al. (2017).

$$L = -\sum_{(h,r,t)\in\mathcal{K}_{train}} \log\left(\frac{\exp(\gamma \cdot s(h,r,t))}{\sum_{t'\in\mathcal{E}} \exp(\gamma \cdot s(h,r,t'))}\right) + \lambda \cdot Reg(h,r,t), \tag{11}$$

where $Reg(h,r,t)$ is the regularization term and $\lambda > 0$ is its factor. Specifically, we only take $Reg(h,r,t)$ as DURA Zhang et al. (2020a) in experiments, since it significantly outperforms other regularization terms. In addition, γ is set to 1 for previous methods and greater than 1 for UniBi. And we set the dimension n to 500. For other details on the implementation, see Appendix E.2.

5.2 MODELING IDENTITY UNIQUELY

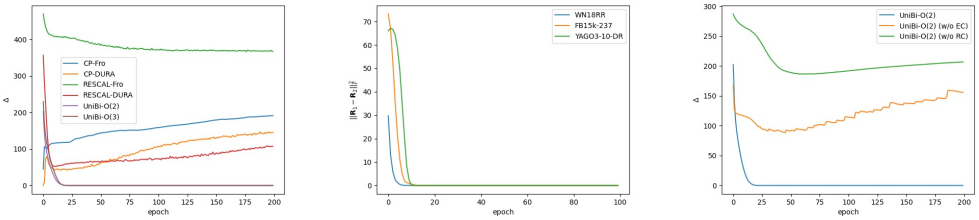
In this part, we verify that 1) UniBi is capable to uniquely model *identity* while previous models fail, and 2) both constraints on the embedding of entities and relations are indispensable. We explicitly add *identity* as a new relation to benchmarks and use its corresponding matrix to determine whether the uniqueness is modeled. In particular, this matrix is supposed to converge to the identity matrix $\mathbf{I}$ or a scaled one. To evaluate it, we introduce a new metric ambiguity degree $\Delta = (\sum_i \frac{\sigma_i}{\sigma_{max}} - 1)^2$.

We first compare UniBi with CP Hitchcock (1927) and RESCAL Nickel et al. (2011), the least and most expressive bilinear model on FB15k-237. Besides, we also apply DURA Zhang et al. (2020a) to models to explore whether these methods are able to uniquely model *identity* under extra regularization. As demonstrated in Fig. 3(a), the ambiguity degree Δ of UniBi converges to 0 while others fails, which verifies that UniBi is capable to uniquely model *identity*. In addition, the ambiguity of other models decrease to some extent when using DURA, yet they are still unable to uniquely model *identity*. Then, to show that UniBi can uniquely converge to *identity*, we use two matrices $\mathbf{R}_1$ and $\mathbf{R}_2$ to model it independently. As shown in Fig. 3(b), the error between $\mathbf{R}_1$ and $\mathbf{R}_2$ also converges to 0, which means that they all converge to $\mathbf{I}$.

We then perform an ablation study to verify that both the entity constraint (EC) and the relation constraint (RC) are needed to model *identity*. The experiments show that only using one constraint is not enough to model the uniqueness of *identity*, as illustrated in Fig. 3(c). And this verify that the existence of problems shown in Fig. 1(a) and Fig. 1(b).

5.3 PERFORMANCE

In this part, we demonstrate that the constraints on UniBi do not lessen the performance. We mainly compared our model with previous SOTA models, i.e. CP Hitchcock (1927), ComplEx Trouillon



(a) UniBi V.S. others.

(b) Error between different matrices converges.

(c) Abaltion of constrains.

Figure 3: UniBi is capable to uniquely model *identity*. (a) the ambiguity degree (Δ) of UniBi converges to 0 while others diverge. (b) The errors between different matrices modeling *identity* converge to 0 on different datasets. (c) Both entity constrain (EC) and relation constrain (RC) are indispensable for UniBi to model *identity*.

Table 2: Evaluation results on WN18RR, FB15k-237 and YAGO3-10-DR datasets. We reimplement RotE, CP, RESCAL, ComplEx with $n = 500$ and denoted by †, while we take results on WN18RR and FB15k-237 from the origin papers and YAGO3-10-DR from Akrami et al. (2020). Best results are in **bold** while the seconds are underlined.

	WN18RR			**FB15K-237**			**YAGO3-10-DR**		
Model	MRR	Hits@1	Hits@10	MRR	Hits@1	Hits@10	MRR	Hits@1	Hits@10
DistMult	0.43	0.39	0.49	0.241	0.155	0.419	0.192	0.133	0.307
ConvE	0.43	0.40	0.52	0.325	0.237	0.501	0.204	0.147	0.315
TuckER	0.470	0.443	0.526	0.358	0.266	0.544	0.207	0.148	0.320
QuatE	0.488	0.438	0.582	0.348	0.248	0.550	-	-	-
RotatE	0.476	0.428	0.571	0.338	0.241	0.533	0.214	0.153	0.332
MurP	0.481	0.440	0.566	0.335	0.243	0.518	-	-	-
RotE	0.494	0.446	**0.585**	0.346	0.251	0.538	-	-	-
CP†	$0.457_{\pm 0.001}$	$0.414_{\pm 0.002}$	$0.549_{\pm 0.003}$	$0.361_{\pm 0.001}$	$0.266_{\pm 0.001}$	$0.551_{\pm 0.001}$	$0.241_{\pm 0.001}$	$0.175_{\pm 0.002}$	$0.370_{\pm 0.003}$
ComplEx†	$0.487_{\pm 0.002}$	$0.445_{\pm 0.001}$	$0.571_{\pm 0.002}$	$0.363_{\pm 0.001}$	$0.269_{\pm 0.001}$	$0.552_{\pm 0.002}$	$0.238_{\pm 0.001}$	$0.174_{\pm 0.002}$	$0.360_{\pm 0.004}$
RESCAL†	$\mathbf{0.495}_{\pm 0.001}$	$\mathbf{0.452}_{\pm 0.002}$	$0.575_{\pm 0.002}$	$0.364_{\pm 0.003}$	$0.272_{\pm 0.003}$	$0.547_{\pm 0.002}$	$0.233_{\pm 0.003}$	$0.168_{\pm 0.004}$	$0.360_{\pm 0.004}$
UniBi-O(2)	$0.487_{\pm 0.002}$	$0.46_{\pm 0.002}$	$0.566_{\pm 0.002}$	$\mathbf{0.370}_{\pm 0.001}$	$\mathbf{0.274}_{\pm 0.001}$	$\mathbf{0.561}_{\pm 0.002}$	$\mathbf{0.247}_{\pm 0.001}$	$0.179_{\pm 0.002}$	$0.376_{\pm 0.002}$
- w/o constraint	$0.488_{\pm 0.001}$	$0.447_{\pm 0.002}$	$0.568_{\pm 0.003}$	$0.361_{\pm 0.001}$	$0.267_{\pm 0.001}$	$0.550_{\pm 0.001}$	$0.242_{\pm 0.001}$	$0.176_{\pm 0.001}$	$0.372_{\pm 0.002}$
UniBi-O(3)	$0.492_{\pm 0.001}$	$\mathbf{0.452}_{\pm 0.001}$	$0.571_{\pm 0.001}$	$0.369_{\pm 0.001}$	$\mathbf{0.274}_{\pm 0.001}$	$0.561_{\pm 0.001}$	$0.246_{\pm 0.001}$	$\mathbf{0.180}_{\pm 0.001}$	$\mathbf{0.377}_{\pm 0.001}$
- w/o constraint	$0.488_{\pm 0.001}$	$0.446_{\pm 0.002}$	$0.567_{\pm 0.003}$	$0.361_{\pm 0.001}$	$0.265_{\pm 0.001}$	$0.550_{\pm 0.001}$	$0.241_{\pm 0.001}$	$0.175_{\pm 0.002}$	$0.370_{\pm 0.003}$

et al. (2016) and RESCAL Nickel et al. (2011) using DURA regularization. Although these models have been implemented by Zhang et al. (2020a), the dimensions of CP and ComplEx are very high and have not been tested on YAGO3-10-DR, so we reimplement them in this paper. In addition, we further remove the constraint of UniBi-O(n) as ablations to eliminate the influence of other factors.

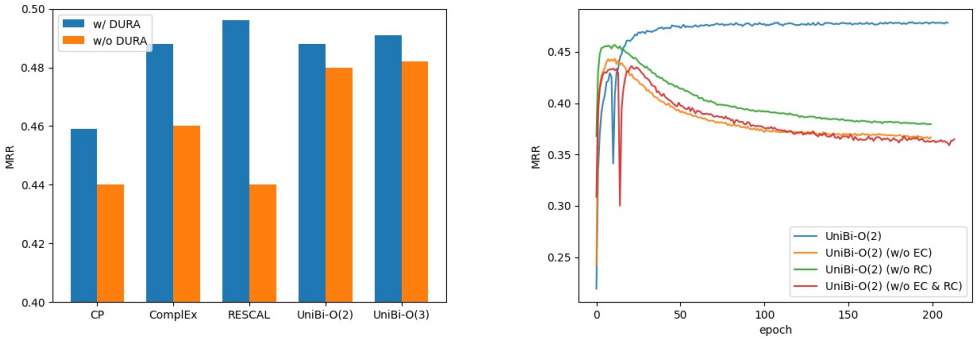
In Tbl. 2, UniBi achieves comparable results to previous bilinear based models and the unconstrained versions. UniBi is only slightly and justifiably below RESCAL on WN18RR, since RESCAL needs require much more time and space[5]. Additionally, UniBi drops on FB15k-237 and YAGO3-10-DR when removing constraints, which shows that the constrains also helps the optimizations.

5.4 Robustness of UniBi

In this part, we demonstrate that UniBi is more robust than previous bilinear based models. We conduct further comparisons without DURA regularization. In addition, we also adopt EC and RC in Section 5.2 to study the effect of constraints on both entity and relation. All experiments are implemented on WN18RR.

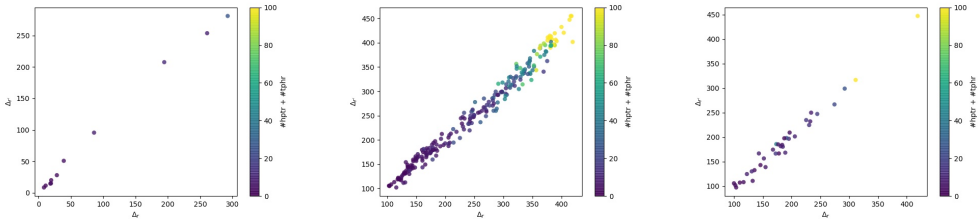
On the one hand, UniBi decreases slightly, while others decrease significantly when the regularization term is removed, as demonstrated in Fig. 4(a). It shows that UniBi is less dependent on extra regularization than other models. On the other hand, we illustrate the MRR metric of UniBi and its ablation models on validation set as epoch grows in Fig. 4(b). It shows that either constrain alleviates overfitting to some extend but fails to prevent the downward sliding behind since the unconstrained part may diverge. Thus, both constraints are verified to be indispensable for the robustness of UniBi.

[5]Detailed in Appendix F.



(a) Ablation of regularization. (b) Ablation of constrains.

Figure 4: UniBi is robust due to the inherent constrains. (a) UniBi maintain its performance without regularization while other models do not. (b) Neither entity constraint (EC) nor relation constrain (RC) alone helps modeling robustness.



(a) WN18RR (b) FB15k-237 (c) YAGO3-10-DR

Figure 5: The ambiguity degree (Δ) and complexity (# hptr + # tphr) of relations in WN18RR, FB15k-237 and YAGO3-10-DR respectively. Two metric are highly correlated and the ambiguity of a relation (Δ_r) and the ambiguity of its reciprocal one ($\Delta_{r'}$) are very close.

5.5 Correlation to Complexity

To verify the statement in Section 4.4.2, we study the connection between the complexity and singular values of each relation on three benchmarks. We evaluate the complexity of a relation by the sum of hptr and tphr. Furthermore, we measure the singular values of a relation by the ambiguity degree Δ. To differentiate Δ of a relation r and its reciprocal relation r', we use Δ_r and $\Delta_{r'}$ to denote them, respectively.

As demonstrated in Fig. 5, we find that singular values are highly correlated with the complexity of a relation. Furthermore, we notice that Δ_r and $\Delta_{r'}$ are very close even if a relation is unbalanced (1-N or N-1), which shows that complexity is handled by aggregation regardless of direction.

6 Conclusion

In this paper, we reveal that previous bilinear models fail to model the uniqueness of relation *identity* required by general frameworks based on group. To address this problem, we analyze its corresponding requirements and propose UniBi, which has been proven to handle it by capturing entities in a unit ball. Furthermore, we demonstrate that UniBi has the inherent regularization from the perspective of Lagrangian function and the interpretability relations from singular values. Experiments verify the above properties and that UniBi is capable to uniquely model *identity* without the cost of performance. Therefore, UniBi fills the gap between the general framework based on groups and specific models in terms of *identity* and paves the way for further studies of both.

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APPENDIX

A PROOFS

A.1 UNIBI IS BOUNDED

Proposition 1. *UniBi is bounded that* $s(h, r, t) \in [-1, 1]$.

Proof. By the Cauchy-Schwarz inequality and the fact that the spectral norm is a generalization of the L2 norm, we have the following.

$$\|\mathbf{h}^\top \mathbf{R}\mathbf{t}\| \leq \|\mathbf{h}^\top \mathbf{R}\|\|\mathbf{t}\| \leq \rho(\mathbf{R})\|\mathbf{h}\|\|\mathbf{t}\| = 1. \tag{12}$$

□

A.2 PROOF OF THEOREM 1

Proof. On the one hand, if $\mathbf{R} = \mathbf{I}$, it is easy to have $\forall \mathbf{h}, \mathbf{t} \in \hat{\mathbb{E}}, \mathbf{h} \neq \mathbf{t}$ that $\mathbf{h}^\top \mathbf{I}\mathbf{h} > \mathbf{h}^\top \mathbf{I}\mathbf{t}$ from the property of cosine.

On the other hand, $\forall \mathbf{R} \in \hat{\mathbb{R}}, \mathbf{R} \neq \mathbf{I}$, we can always give a counterexample. Using singular value decomposition (SVD), we have $\mathbf{R} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$, where $\Sigma = \text{Diag}[\sigma_1, \ldots, \sigma_n]$ with $\sigma_i \geq 0$ and U, V are orthogonal matrices. Since $\rho(\mathbf{R}) = 1$, we have $\sigma_{max} = \max(\sigma_i) = 1$.

Besides, we notice that since U, V are orthogonal matrices that do not change the norm of vectors, we have $\|\mathbf{h}^\top \mathbf{U}\| = \|\mathbf{V}^\top \mathbf{t}\| = 1$ and use $\hat{\mathbf{h}}$ and $\hat{\mathbf{t}}$ to denote $\mathbf{U}^\top \mathbf{h}$ and $\mathbf{V}^\top \mathbf{t}$ for mathematical simplicity. We consider three scenarios and discuss them separately.

(1) If all singular values of $\mathbf{R}$ are equivalent, we have $\mathbf{\Sigma} = \mathbf{I}$, and we have:

$$s(h, r, t) = \mathbf{h}^\top \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top \mathbf{t} = \hat{\mathbf{h}}^\top \mathbf{I}\hat{\mathbf{t}} = \hat{\mathbf{h}}^\top \hat{\mathbf{t}}. \tag{13}$$

It is easy to notice that the above equation just goes back to the cosine function, and it has the maximum value when $\hat{\mathbf{h}} = \hat{\mathbf{t}}$ and $\mathbf{U}^\top \mathbf{h} = \mathbf{V}^\top \mathbf{t}$. If $\mathbf{U}\mathbf{V}^\top = \mathbf{I}$, this contradicts the assumption that $\mathbf{R} \neq \mathbf{I}$. If $\mathbf{U}\mathbf{V}^\top \neq \mathbf{I}$, then we have $\mathbf{h} \neq \mathbf{t}$, since $\mathbf{h} = (\mathbf{U}^\top)^{-1}\mathbf{V}^\top \mathbf{t} = \mathbf{U}\mathbf{V}^\top \mathbf{t}$. It means $\mathbf{h}^\top \mathbf{R}\mathbf{h} < \mathbf{h}^\top \mathbf{R}\mathbf{t}$ in this situation.

(2) If not all singular values of $\mathbf{R}$ are equivalent and $\mathbf{U} = \mathbf{V}$, there $\exists i, j \in 1, \ldots, n$ that $\sigma_i \neq \sigma_j$. It may be assumed that $\sigma_i > \sigma_j$. Then we take $\forall \mathbf{h} \in \hat{\mathbb{E}}$ that has $\hat{\mathbf{h}}_j = (\frac{\sigma_i}{\sigma_j} - \epsilon)\hat{\mathbf{h}}_i$ where $\epsilon \in (0, \frac{\sigma_i}{\sigma_j} - 1)$. Then we take

$$\hat{\mathbf{t}}_k = \begin{cases} \hat{\mathbf{h}}_k, & k \neq i, j, \\ \hat{\mathbf{h}}_j, & k = i, \\ \hat{\mathbf{h}}_t, & k = j. \end{cases} \tag{14}$$

It is easy to notice that $\hat{\mathbf{h}} = \mathbf{U}^\top \mathbf{h}, \hat{\mathbf{t}} = \mathbf{U}^\top \mathbf{t}$ and $\mathbf{h} \neq \mathbf{t}$, then we have

$$\begin{aligned} \mathbf{h}^\top \mathbf{R}\mathbf{t} &= \mathbf{h}^\top \mathbf{U}\mathbf{R}\mathbf{U}^\top \mathbf{t} \\ &= \hat{\mathbf{h}}^\top \mathbf{\Sigma}\hat{\mathbf{t}} \\ &= \sigma_i \hat{\mathbf{h}}_i \hat{\mathbf{t}}_i + \sigma_j \hat{\mathbf{h}}_j \hat{\mathbf{t}}_j + \sum_{k \neq i,j} \sigma_k \hat{\mathbf{h}}_k \hat{\mathbf{t}}_k \\ &= \sigma_i \hat{\mathbf{h}}_i \hat{\mathbf{h}}_j + \sigma_j \hat{\mathbf{h}}_j \hat{\mathbf{h}}_i + \sum_{k \neq i,j} \sigma_k \hat{\mathbf{h}}_k^2, \end{aligned} \tag{15}$$

similarly, we have

$$\begin{aligned}\mathbf{h}^\top\mathbf{R}\mathbf{h} &= \mathbf{h}^\top\mathbf{U}\mathbf{R}\mathbf{U}^\top\mathbf{h} \\ &= \hat{\mathbf{h}}^\top\mathbf{\Sigma}\hat{\mathbf{h}} \\ &= \sigma_i\hat{\mathbf{h}}_i^2 + \sigma_j\hat{\mathbf{h}}_j^2 + \sum_{k\neq i,j}\sigma_k\hat{\mathbf{h}}_k^2.\end{aligned} \tag{16}$$

Then, we use Eq. equation 16 minus Eq. equation 15, and we have

$$\begin{aligned}&\mathbf{h}^\top\mathbf{R}\mathbf{h} - \mathbf{h}^\top\mathbf{R}\mathbf{t} \\ =&\left(\sigma_i\hat{\mathbf{h}}_i^2 + \sigma_j\hat{\mathbf{h}}_j^2 + \sum_{k\neq i,j}\sigma_k\hat{\mathbf{h}}_k^2\right) - \left(\sigma_i\hat{\mathbf{h}}_i\hat{\mathbf{h}}_j + \sigma_j\hat{\mathbf{h}}_j\hat{\mathbf{h}}_i + \sum_{k\neq i,j}\sigma_k\hat{\mathbf{h}}_k^2\right) \\ =&\sigma_i(\hat{\mathbf{h}}_i^2 - \hat{\mathbf{h}}_i\hat{\mathbf{h}}_j) + \sigma_j(\hat{\mathbf{h}}_j^2 - \hat{\mathbf{h}}_i\hat{\mathbf{h}}_j) \\ =&\sigma_i\hat{\mathbf{h}}_i(\hat{\mathbf{h}}_i - \hat{\mathbf{h}}_j) - \sigma_j\hat{\mathbf{h}}_j(\hat{\mathbf{h}}_i - \hat{\mathbf{h}}_j) \\ =&(\sigma_i\hat{\mathbf{h}}_i - \sigma_j\hat{\mathbf{h}}_j)(\hat{\mathbf{h}}_i - \hat{\mathbf{h}}_j) \\ =&\left(\sigma_i\hat{\mathbf{h}}_i - \sigma_j(\frac{\sigma_i}{\sigma_j} - \epsilon)\hat{\mathbf{h}}_i\right)\left(\hat{\mathbf{h}}_i - (\frac{\sigma_i}{\sigma_j} - \epsilon)\hat{\mathbf{h}}_i\right) \\ =&\left(\sigma_i\hat{\mathbf{h}}_i - \sigma_i\hat{\mathbf{h}}_i + \epsilon\sigma_j\hat{\mathbf{h}}_i\right)\left(1 - \frac{\sigma_i}{\sigma_j} + \epsilon\right)\hat{\mathbf{h}}_i \\ =&\epsilon\sigma_j\hat{\mathbf{h}}_i^2(1 - \frac{\sigma_i}{\sigma_j} + \epsilon) \\ <&0,\end{aligned} \tag{17}$$

which means that $\mathbf{h}^\top\mathbf{R}\mathbf{h} < \mathbf{h}^\top\mathbf{R}\mathbf{t}$ in this case.

(3) If not all singular values of $\mathbf{R}$ are equivalent and $\mathbf{U} \neq \mathbf{V}$, there exists $k \in 1, \ldots, n$ such that $\sigma_k = \sigma_{max} = 1$ since $\rho(\mathbf{R}) = 1$. Then we take the following.

$$\hat{\mathbf{h}}_i = \hat{\mathbf{t}}_i = \begin{cases}1, & i = k, \\ 0, & i \neq k.\end{cases} \tag{18}$$

It should be noted that $\hat{\mathbf{h}} = \hat{\mathbf{t}}$ and $\mathbf{h} \neq \mathbf{t}$ since $\mathbf{U} \neq \mathbf{V}$. Then, we have

$$\begin{aligned}\mathbf{h}^\top\mathbf{R}\mathbf{t} &= \mathbf{h}^\top\mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top\mathbf{t} \\ &= \hat{\mathbf{h}}^\top\mathbf{\Sigma}\hat{\mathbf{t}} \\ &= \sigma_k \\ &= 1.\end{aligned} \tag{19}$$

Since Proposition 1 proves that UniBi is bounded by $[-1, 1]$, we have $\mathbf{h}^\top\mathbf{R}\mathbf{h} \leq 1 = \mathbf{h}^\top\mathbf{R}\mathbf{t}$, which means that $s(h, r, h) > s(h, r, t)$ does not always hold.

In summary, we can conclude that UniBi has $\mathbf{h} \neq \mathbf{t},\ \mathbf{h}^\top\mathbf{R}\mathbf{h} > \mathbf{h}^\top\mathbf{R}\mathbf{t}$ iff. $\mathbf{R} = \mathbf{I}$, which means that UniBi can model *identity* uniquely in terms of definition 4.

□

A.3 Proof of Theorem 2

Proof. if we have $\|\mathbf{e}\| = 1, \rho(\mathbf{R}) = 1$. The equation for the entity part obviously holds, and by Proposition 1, we have the following.

$$\|\mathbf{R}\mathbf{e}\| \leq \rho(\mathbf{R})\|\mathbf{e}\| = \rho(\mathbf{R}) = 1, \tag{20}$$

similarly, we have $\|\mathbf{e}^\top\mathbf{R}\| \leq 1$.

Moreover, such condition will become necessary and sufficient if $\exists\hat{e}$ that either either $\|\hat{\mathbf{e}}^\top\mathbf{R}\| = 1$ or $\|\mathbf{R}\hat{\mathbf{e}}\| = 1$.

To prove it, if we have $\|\mathbf{e}^\top \mathbf{R}\| \leq 1$ and $\|\mathbf{R}\mathbf{t}\| \leq 1$, we use SVD to any $\mathbf{R}$ and gets $\mathbf{R} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}$. Then, we denote $\sigma = Diag(\sigma)$ where σ is the vector of singular values, and we have $\forall \mathbf{e}, \|\sigma \cdot \mathbf{e}\| \leq 1$.

If $\exists i, \sigma_i > 1$, we take $i \neq j, e_i = 1, e_j = 0$ to show that $\|\mathbf{e} \cdot \sigma\|$ is larger than 1. Therefore, we have $\forall i, \sigma_i \leq 1$. Moreover, if $\forall i, 0 < \sigma_i < 1$, we take $\bar{\mathbf{e}} = \mathbf{V}\hat{\mathbf{e}}$

$$\|\sigma \cdot \bar{\mathbf{e}}\|^2 = \sum_i \sigma_i^2 \bar{e}_i^2 < \sigma_i \bar{e}_i^2 = 1, \tag{21}$$

which also violates that $\|\mathbf{R}\mathbf{e}\| = \|\mathbf{\Sigma}\mathbf{V}\hat{\mathbf{e}}\| = \|\sigma \cdot \bar{\mathbf{e}}\| = 1$. Therefore, there $\exists k, \sigma_k = 1$ and we have $\rho(\mathbf{R}) = 1$.

□

A.4 Proof of Proposition 2

Proof. If a relation r is invertible, it means there exists an inverse relation r^{-1} that ensure $r \circ r^{-1} = r^{-1} \circ r = identity$, where $\circ$ is the composition of relations. Consider that *identity* relation means that no different entities will appear in a triple under it, or KGs only contain triples like $\forall e \in \mathcal{E}, (e, identity, e)$.

Consider a complex relation that has multiple tail entities for a head entity, that is, $\exists h, t_1, t_2\ (h, r, t_1), (h, r, t_2)$. In order to remap the entities t_1 and t_2 back to h, the inverse relation r^{-1} has to contain triples that $(t_1, r^{-1}, h), (t_2, r^{-1}, h)$. Although $r \circ r^{-1}$ could map h to h, $r^{-1} \circ r$, it fails to map t_1, t_2 back to themselves separately since both $(t_1, r^{-1} \circ r, t_1)$ and $(t_1, r^{-1} \circ r, t_2)$ are true. Similarly, if a relation has multiple heads, we can also obtain the above conclusion.

Therefore, all complex relations are inherently non-invertible.

□

B Discuss of Distance Based models

We mention that distance based model could model *identity* uniquely, and here we give its corresponding proof. Here, we only consider models that can be written in the basic form of $s(h, r, t) = -\|\mathbf{R}\mathbf{h} - \mathbf{t}\|$. Note that translation is also considered in such a form if we take translation as a linear transformation. Furthermore, the model must ensure that $\mathbf{I} \in \hat{\mathbb{R}}$ and $\hat{\mathbb{E}} = \mathbb{R}^n$. Other peculiar scenarios are not considered in this discussion.

Theorem 3. *A distance based model $s(h, r, t) = -\|\mathbf{R}\mathbf{h} - \mathbf{t}\|$ with $\mathbf{I} \in \hat{\mathbb{R}}$ and $\hat{\mathbb{E}} = \mathbb{R}^n$ can model identity uniquely.*

Proof. On the one hand, if $\mathbf{R} = \mathbf{I}$, it is easy to have

$$-\|\mathbf{R}\mathbf{h} - \mathbf{t}\| = -\|\mathbf{h} - \mathbf{t}\| \leq -\|\mathbf{h} - \mathbf{h}\| = 0, \tag{22}$$

where $\mathbf{h} \neq \mathbf{t}$.

On the other hand, if $\mathbf{R} \neq \mathbf{I}$, if $\mathbf{R}$ is not a singular matrix, we take $\mathbf{t} = \mathbf{R}\mathbf{h}$ and have

$$-\|\mathbf{R}\mathbf{h} - \mathbf{h}\| \leq 0 = -\|\mathbf{R}\mathbf{h} - \mathbf{R}\mathbf{h}\| = -\|\mathbf{R}\mathbf{h} - \mathbf{t}\|. \tag{23}$$

□

Therefore, we prove that distance-based models are born to uniquely model *identity*.

C Comparison to previous restrictions

Although it is true that entity normalization and set $\mathbf{R}$ to orthogonal matrices, which is a special case of $\rho(\mathbf{R}) = 1$, are common in KGE models, our constraint differs from their approach as follows.

(1) the constraint for relation based on the spectral radius, i.e., $\rho(\mathbf{R}) = 1$, is first proposed in our work, which is indispensable and irreplaceable to model the *identity* uniquely without the cost of

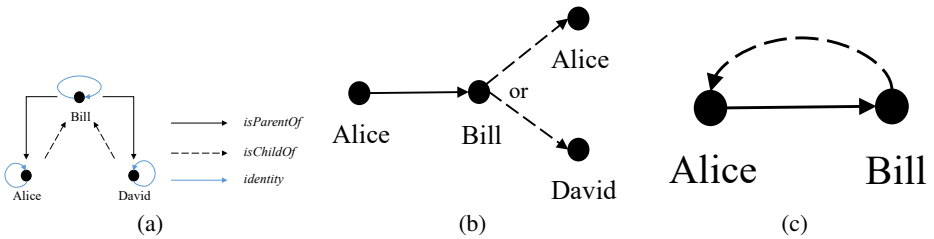


Figure 6: Why some relations are non-invertible. (a) A toy example. (2) True case. (3) False case.

the performance. If we set $\mathbf{R}$ to be orthogonal while keeping the normalization of entities, the performance will drop significantly, e.g., MRR: 0.488 $\rightarrow$ 0.471 for UniBi-O(2) on WN18RR.

(2) Only the combination of entity and relation constraints succeeds to model *identity* uniquely, as shown in Figure 3(c). It suggests that constraints on entity and relation should be treated as a whole rather than a combination of two unrelated things.

(3) At first glance our constraint looks very similar to that of TransR Lin et al. (2015), but in fact there is a big difference. The TransR's constraint is $\|\mathbf{h}\| \leq 1$, $\|\mathbf{h}\mathbf{M}_r\| \leq 1$, and $\|\mathbf{t}\mathbf{M}_r \leq 1$, and has three differences from ours.

i) For TransR, $\|\mathbf{h}\mathbf{M}_r\| \leq 1$ and $\|\mathbf{t}\mathbf{M}_r\| \leq 1$ is the constraint **itself**. In contrast, $\mathbf{R}^\top\mathbf{h} \leq 1$ and $\mathbf{R}\mathbf{t} \leq 1$ is **deduction** of our constraints $\|\mathbf{e}\| = 1$ and $\rho(\mathbf{R}) = 1$.

ii) TransR does not normalize the entities, and we have shown in Fig. 1(a) that normalization is necessary for a bilinear based method to uniquely model *identity*.

iii) TransR is a distance based model, and as we have shown in Appendix B, distance based models do not need to consider the problem of *identity*, thus the proposal of TransR is difference to us.

Therefore, we believe that our combination of constraints is novel, since it proposes a new constraint for the relation, and the two parts are deliberately rather than arbitrarily combined.

D From Group to Monoid

Since the singular values are less than or equal to 1, some matrices do not have their corresponding inverse elements in $\hat{\mathbb{R}}$. Therefore, UniBi violates the definition of group, which requires that each element has its inverse element inside. However, we argue that some relations are inherently non-invertible and misidentified by previous work Yang et al. (2020); Sun et al. (2019); Xu & Li (2019).

For example, in Fig. 6(a), if two relations are inverse elements of each other, their composition must be *identity*. However, we find the combination of *IsParentOf* and *IsChildOf* is not the *identity*, since the child of Alice's parent is "Alice or David" rather than "Alice itself" as demonstrated in Fig. 6(b) and Fig. 6(c).

It should be noted that we are not saying that these two relations are irrelevant, but rather pointing out that their combination does not strictly fit our definition of *identity*. Moreover, the fact that they are both **non-invertible** does not mean that they cannot form the **inversion pattern** Sun et al. (2019), since definitions of the two concepts are different and do not conflict.

Beyond the specific example, we generalize it to all complex relations that appear in both triples (e_1, r, e_2) and (e_1, r, e_3) (or (e_3, r, e_2)), where $e_1, e_2, e_3 \in \mathcal{E}$, and $e_1 \neq e_2 \neq e_3$. Furthermore, we have the following proposition.

Proposition 2. *$\forall r \in \mathcal{R}$, if r is a complex relation, then r is non-invertible.*

Proof. Please refer to Appendix A.4. □

Table 3: Hyperparameters found by grid search. λ is the regularization coefficient, γ is the scaling factor, b is the batch size.

	WN18RR			**FB15K237**			**YAGO3-10-DR**		
Model	λ	γ	b	λ	γ	b	λ	γ	b
CP	1e-1	1	100	5e-2	1	100	5e-3	1	1000
ComplEx	1e-1	1	100	5e-2	1	100	1e-2	1	1000
RESCAL	1e-1	1	1000	5e-2	1	1000	5e-2	1	1000
UniBi-O(2)	2	20	100	2	25	1000	1.5	30	1000
- w/o constraint	1e-1	1	100	5e-2	1	1000	5e-2	1	1000
UniBi-O(3)	2	15	100	1.5	20	1000	1.5	30	1000
- w/o constraint	1e-1	1	100	5e-2	1	1000	5e-2	1	1000

Since these non-invertible relations extensively present in KGs, the requirement that each element has its inverse element in the set should be abandoned. Thus, rather than group, we think monoid is a better structure for relations by their definitions[6].

E Implement Details

E.1 Rotation Matrices of UniBi

In Section 5, we propose two variants of UniBi, i.e., UniBi-O(2) and UniBi-O(3). Here, we give the rotation matrix $\mathbf{SO}(k)$ they used specifically.

$$\mathbf{SO}(2) = \begin{bmatrix} x & -y \\ y & x \end{bmatrix}, \ \mathbf{SO}(3) = \begin{bmatrix} p & -q & -u & -v \\ q & p & v & -u \\ u & -v & p & q \\ v & u & -q & p \end{bmatrix}, \tag{24}$$

where $x, y, p, q, u, v \in \mathbb{R}$ and $x^2 + y^2 = 1, p^2 + q^2 + u^2 + v^2 = 1$.

E.2 Hyperparameters

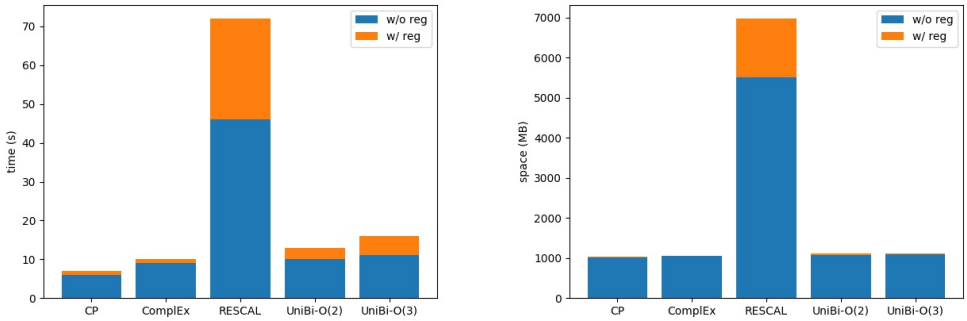
We fix the dimension of all models except RESCAL on WN18RR to 500, while RESCAL on WN18RR is set to 256 following Zhang et al. (2020a). We choose Adam Kingma & Ba (2015) as the optimizer and fix the learning rate at $1e-3$. We set the maximum epochs to 200 and apply the early stopping strategy.

We set the scaling factor γ to 1 for all models except UniBi. And we search γ from $\{1, 5, 10, 15, 20, 25, 30\}$ for UniBi. For the factor for regularization λ we search $\{1, 5e-1, 1e-1, 5e-2, 1e-2, 5e-3, 1e-3\}$ for all models except UniBi and $\{0.5, 1, 1.5, 2, 2.5, 3\}$ for it. Furthermore, we do not search for λ_1 and λ_2 in Eq. equation 10 as in the original paper of DURA Zhang et al. (2020a). we adopt their settings and set $\lambda_1 = 0.5, \lambda_2 = 1.5$ for ComplEx Trouillon et al. (2016) and CP Hitchcock (1927), while $\lambda_1 = \lambda_2 = 1$ for other cases. The search results are listed on the Tbl. 3. We search for the batch size from $\{100, 1000\}$.

In addition, we implemented all the experiments in PyTorch with a single NVIDIA GeForce RTX 1080Ti graphics card. We repeat each experiment five times and take their means and standard deviations.

For the experiments in Section 5.4, we set γ for UniBi without DURA in Section 5.4 to $10, 15, 25$ for WN18RR, FB15k-237 and YAGO3-10-DR for UniBi, respectively.

[6]Definition 1 and Definition 2.



(a) Comparison of time.

(b) Comparison of space.

Figure 7: UniBi takes a little more time than other models with linear parameters (CP and ComplEx) and significantly efficient than ones with quadratic parameters (RESCAL).

F TIME AND SPACE COMPLEXITY

Since UniBi needs to calculate some constraints, it spends more space and time. Here, we compare the time and space consumption of UniBi and CP, ComplEx, and RESCAL on FB15k 237, and set the batch size to 1000.

As demonstrated in Fig. 7(a) and Fig. 7(b), UniBi takes a little more time than CP and ComplEx, and more time to compute the regularization since it is more complex. Nevertheless, we noticed that UniBi occupies a space similar to that of CP and ComplEx.

In addition, we note that in Section5.3, UniBi outperforms all bilinear based models except RESCAL on WN18RR. And RESCAL needs significantly more time and space than other models. Therefore, it is not as efficient as other models.

In summary, although UniBi takes a little more time, it is a good balance between complexity and performance.

In future work, we will consider finding other constraints on the relation instead of the spectral radius.