DisenE: Disentangling Knowledge Graph Embeddings

Xiaoyu Kou
Yankai Lin
Yuntao Li
Jiahao Xu
Peng Li
Jie Zhou
Yan Zhang

1Key Laboratory of Machine Perception (MOE), Department of Machine Intelligence, Peking University, Beijing, China
2Pattern Recognition Center, WeChat AI, Tencent Inc., China

{kouxiaoyu,li.yt,xujiahao,zhyzhy001}@pku.edu.cn
{yankailin,patrickpli,withtomzhou}@tencent.com

Abstract

Knowledge graph embedding (KGE), aiming to embed entities and relations into low-dimensional vectors, has attracted wide attention recently. However, the existing research is mainly based on the black-box neural models, which makes it difficult to interpret the learned representation. In this paper, we introduce DisenE, an end-to-end framework to learn disentangled knowledge graph embeddings. Specially, we introduce an attention-based mechanism that enables the model to explicitly focus on relevant components of entity embeddings according to a given relation. Furthermore, we introduce two novel regularizers to encourage each component of the entity representation to independently reflect an isolated semantic aspect. Experimental results demonstrate that our proposed DisenE investigates a perspective to address the interpretability of KGE and is proved to be an effective way to improve the performance of link prediction tasks. The code and datasets are released on https://github.com/KXY-PUBLIC/DisenE.

1 Introduction

Recently, knowledge graph embedding (KGE) models which represent entities and relations of KGs in semantic vector space have drawn wide attention from both academic and industry. The goal of KGE is to find a useful representation for different downstream tasks such as link prediction (Bordes et al., 2013) and question answering (Bordes et al., 2014). Intuitively, explainable representation can help researchers analysis current models and place more trust in it. However, most existing KGE works, whether reconstruction-based (Bordes et al., 2013; Dettmers et al., 2018) or bilinear-based (Nguyen et al., 2018; Balazevic et al., 2019), ignore the necessary of interpretable representations. The black-box nature makes it difficult to understand the learned embeddings and let alone explain them in an intuitive manner, which largely wipes out the rich interpretability for KGs itself.

To address this issue, we study the problem of disentangling KGE. In real-world KGs, entities are supposed to carry rich information, which can be compressed into multiple components. This provides us a perspective to disentangle entity embeddings. As the example in Figure 1(a), the entity “David Beckham” may contain several components, such as “Characteristic”, “Family”, “Work”, etc. For relations “country” or “lived_in”, “David Beckham” should focus on component “Places”; while for the relation “team_of”, “David Beckham” should pay more attention to “Work” component. Some previous works (Wang et al., 2014; Lin et al., 2015) consider this by projecting entity representations into relation-specific semantic space, but the representations themselves are still not disentangled.

In this work, we propose an end-to-end framework DisenE to learn disentangled KG embeddings. Specifically, DisenE divides entity embedding into multiple independent components and employs attention mechanism to explicitly capture relevant components of the entity according to the given relation. To force each component to independently reflect an isolated semantic aspect, we introduce two novel regularizers to effectively incorporate relation constraints. Note that our proposed framework is general enough to be applicable to most existing KGE methods, such as reconstruction-based or bilinear-based, to obtain the local correlation of the triplet under each component. Extensive experiments indicate that

*This work is done when Xiaoyu Kou was interning at Pattern Recognition Center, WeChat AI, Tencent Inc, China
DisenE can achieve competitive performance over previous strong baselines on link prediction task. In addition, we provide a case study to offers some insights of disentangled entity embeddings.

The contribution of this paper is not only the design of the proposed framework, but also provides a new perspective to address the interpretability of KGE, which is important for downstream applications and not fully explored yet in the KG community. The inherently more interpretable embeddings learned by our DisenE model can potentially facilitate debugging and auditing (Lipton, 2018), which can further improve the robustness of KGE models. Hence, we hope to inspire researchers to notice the meaningness of disentangling KG embeddings.

2 Related Work

In recent years, there are a large number of knowledge graph embedding (KGE) models have been proposed, which mainly represent entities and relations with low-dimensional vectors or matrices. One line of work operates in a reconstructive way. They reconstruct the embedding of head (or tail) using the corresponding relation and tail (or head) embeddings, and calculate the plausibility of the triplet by measuring the difference between the original and the reconstructed embeddings. These works either model this relationship in an explainable way (e.g., TransE (Bordes et al., 2013), RotatE (?)), or utilize the black-box but expressive convolution operations (e.g., ConvE (Dettmers et al., 2018)). Another line of work considers link prediction as a semantic matching problem (Ji et al., 2020). They take the embeddings of the head, relation and tail as input, and output a semantic matching score for the elements in each triplet using bi-linear transformation (e.g., DistMult (Yang et al., 2014), ComplEx (Trouillon et al., 2016), SimplE (Kazemi and Poole, 2018)), convolution (e.g., ConvKB (Nguyen et al., 2018)), CapsE (Vu et al., 2019), KBGAT (Nathani et al., 2019) and etc.

The existing KG embedding methods, however, cannot learn disentangled representations. In fact, few previous works (Wang et al., 2014; Lin et al., 2015) do notice that different relations have different effects on the representation of entities, so they translate entity representation into relation space by adopting projection vectors or matrices. Yet they fail to isolate each independent factor and therefore cannot disentangle the representation of entities. Though disentangled factor learning has received intensive attention in computer vision (Higgins et al., 2017; Alemi et al., 2017), how to learn disentangled embeddings for a knowledge graph remains largely unexplored. In this paper, we study the disentanglement of factors behind the formation of knowledge graphs and present DisenE, which can directly and explicitly discover which component of the entity is more relevant to a given relation.

3 Disentangled Knowledge Graph Embeddings

Notations Let $\mathcal{E}$, $\mathcal{R}$ denote the entity set and the relation set presented in a knowledge graph $G$, where $G$ can be formalised as a set of triplets \{\( (h, r, t) \) \} $\subseteq \mathcal{E} \times \mathcal{R} \times \mathcal{E}$. Given a triplet \( (h, r, t) \), we denote their embeddings as \( h, t \in \mathbb{R}^d \) and \( r \in \mathbb{R}^l \). Knowledge graph embedding (KGE) models usually learn entity and relation embeddings by maximizing a score function $f(h, r, t)$ over observed facts, which is expected to give higher scores for valid triplets than invalid ones.
We evaluate our DisenE model on two widely-used benchmark datasets: WN18RR (Dettmers et al., 2018) and FB15k-237 (Toutanova and Chen, 2015). These two datasets are created to avoid reversible relation problems, which makes the link prediction task more realistic and challenging (Toutanova and Chen, 2015). The statistics of WN18RR and FB15k-237 are presented in Table 1.

**Methodology** The idea of DisenE is to decouple the rich information of an entity into several components, where different triplets will involve with different components. To this end, we learn a disentangled entity embedding $e$ which composed of $K$ independent components, i.e., $e = [e^1, e^2, ..., e^K]$, where $e^k \in \mathbb{R}^d$ is used to represent the aspect of entity $e$ that are pertinent to factor $k$.

The overall architecture of DisenE is shown in Figure 1(b). For a triplet $(h, r, t)$, we aim to employ an attention layer to explicitly extract relevant components of $h$ and $t$ according to the relation $r$. Specially, we first calculate the attention value to the $k$-th component of the head and tail entity embeddings by performing a non-linearity transformation over the concatenation of entity and relation:

$$a^k = \text{ReLU}(W_1[h^k; r; t^k]), \quad \alpha^k = \frac{\exp(a^k)}{\sum_{j=1}^K \exp(a^j)},$$  \hspace{1cm} (1)

where $W_1 \in \mathbb{R}^{1 \times 3d}$ is a trainable matrix ($l = \frac{d}{K}$); $[; ; ]$ denotes the concatenation operation; $a^k$ scores how much the relation is related to the $k$-th components of the head and tail entities; $\alpha^k$ is a relative attention value achieved by applying a softmax operation over $a^k$.

After that, we can leverage exiting KGE methods to extract the local correlation of $h^k$, $r$ and $t^k$. As described in the introduction, KGE models can mainly be divided into two categories: reconstruction-based and bilinear-based models. We explore the generalization ability of our framework and leverage two classic KGE models including TransE (reconstruction-based) and ConvKB (bilinear-based):

$$\text{TransE} : \alpha^k = [h^k; r; t^k], \quad \text{ConvKB} : \alpha^k = \text{ReLU}(\text{Conv}([h^k; r; t^k]),$$  \hspace{1cm} (2)

where Conv$(\cdot)$ indicates the convolutional layer with $M$ filters, and $\alpha^k \in \mathbb{R}^{Md/K}$ is the output representation of the $k$-th component.

Finally, we define the score function $f(h, r, t) = W_2 \left( \sum_{k=1}^K \alpha^k o^k \right)$, where $W_2$ is a normalization operation when we leverage TransE; and $W_2 \in \mathbb{R}^{1 \times \frac{Md}{K}}$ is a trainable matrix when using ConvKB.

**Learning** We utilize soft-margin loss to train our DisenE model:

$$\mathcal{L}_{\text{triplet}} = \sum_{(h, r, t) \in G \cup G'} \log \left( 1 + \exp \left( y_{(h, r, t)} \cdot f(h, r, t) \right) \right),$$  \hspace{1cm} (3)

where $G'$ indicate a set of invalid triplets, $y_{(h, r, t)} = 1$ if $(h, r, t) \in G$, otherwise, $y_{(h, r, t)} = -1$.

To force each component of the representations to independently reflect an isolated semantic aspect, we introduce two novel regularizers. (1) $\mathcal{L}_{\text{REL}_1}$: a relation will pay attention to the same component for different entities. For each triplet $(h, r, t) \in G$, we sample a set $T(h, r, t) \in G$ of $N$ triplets that have relation $r$. Then we apply a constraint on the disentangled attention values for these triplets by minimizing their KL distance. (2) $\mathcal{L}_{\text{REL}_2}$: the fewer components a relation focuses on, the better the entanglement effect. We encourage the sum of the attention values of the top-$m$ selected components to reach 1. Formally, two regularizers are defined as:

$$\mathcal{L}_{\text{REL}_1} = \sum_{(h, r, t) \in G} \sum_{(h', r', t') \in T(h, r, t)} \frac{1}{N} \text{D}_{KL}(\alpha(h, r, t); \alpha(h', r', t')), \quad \mathcal{L}_{\text{REL}_2} = \sum_{(h, r, t) \in G} (1 - \sum_{i} \alpha^i).$$  \hspace{1cm} (4)

Therefore, the overall loss function of our proposed model is: $\mathcal{L} = \mathcal{L}_{\text{triplet}} + \beta \cdot \mathcal{L}_{\text{REL}_1} + \eta \cdot \mathcal{L}_{\text{REL}_2}$, where $\beta$ and $\eta$ indicate the weight of $\mathcal{L}_{\text{REL}_1}$ and $\mathcal{L}_{\text{REL}_2}$ respectively.

### 4 Experiments

#### 4.1 Datasets

We evaluate our DisenE model on two widely-used benchmark datasets: WN18RR (Dettmers et al., 2018) and FB15k-237 (Toutanova and Chen, 2015). The statistics of WN18RR and FB15k-237 are presented in Table 1.
Table 1: Statistics of experimental datasets.

| Dataset      | |E| | |R| | Train | Valid | Test |
|--------------|---|---|---|---|---|---|---|
| WN18RR       | 40,943 | 11 | 86,835 | 3,034 | 3,134 |
| FB15k-237    | 14,541 | 237 | 272,115 | 17,535 | 20,466 |

4.2 Experimental Settings

We use Adam (Kingma and Ba, 2014) with the initial learning rate set at 0.001 as the optimizer and fine-tune the hyper-parameters on the validation dataset. We perform a grid search for the hyper-parameters specified as follows: the number of components $K \in \{2, 4, 6, 8, 10\}$, relation embedding dimension $l \in \{100, 200\}$ (note that entity embedding dimension $d = K \times l$), batch size $b \in \{128, 256\}$, sample size of $L_{REL} = N \in \{10, 50, 100\}$, the number of selected components $m \in \{1, 2, 4\}$ and the number of filters $M \in \{50, 100\}$ with filter size $3 \times 3$. We found that the following combination of hyper-parameters works well on both datasets: $K = 6$, $l = 100$, $b = 128$, $N = 50$, $m = 2$, $M = 50$. Following existing works (Bordes et al., 2013), the evaluation metrics include mean rank (MR), mean reciprocal rank (MRR), and the proportion of valid test triplets in the top $N$ ranks (H@$N$) for $N = 1, 3$ and 10.

4.3 Main Results

We compare our DisenE model with previous state-of-the-art KGE models, including reconstruction-based models TransE (Bordes et al., 2013), ConvE (Dettmers et al., 2018), RotatE (?) and bilinear-based models ComplEx (Trouillon et al., 2016), ConvKB (Nguyen et al., 2018), TuckER (Balazevic et al., 2019), KBGAT (Nathani et al., 2019), to empirically show the effectiveness of disentangled KGE for the link prediction task.

From Table 2, we find that: (1) Our DisenE model does better than the closely related models TransE and ConvKB on both experimental datasets, especially on FB15k-237 where DisenE (ConvKB) gains improvements on almost all the metrics. It verifies the effectiveness of our disentangled approach in the link prediction task. (2) We can see that DisenE (ConvKB) achieves the best results on FB15k-237 and best MR score on WN18RR, which indicating that a disentangled approach tends to rank higher for all the ground-truth triplets than other methods. (3) Compared to the results on WN18RR, the improvement in FB15k-237 is more significant. The reason is that the phenomenon of containing multiple semantic components is more significant in the KG that contains a large number of relations. As a result, our model can capture a more compact and solid structure on FB15k-237 benchmark.

4.4 Sensitivity Study

In this section, we investigate the sensitivity of the number of components $K$ under different experimental methods. We use $l = 100$, $b = 128$, $M = 50$ to run our DisenE with five different $K$ settings. The results on FB15k-237 are reported in Figure 2(b) and the results of WN18RR are presented in Appendix A.

From the figures, we find that as the number of $K$ increases, DisenE starts to achieve better performance, which emphasizes the importance of disentangling on a large number of relations. However, when $K$ is very large, i.e., $K > 6$ in DisenE (ConvKB), additional components not only consume more computing resources, but also have a negative effect on performance. This is because entities don’t have too many semantic aspects in this dataset, most of the useful information can be classified into several components.

4.5 Case Study

In this section, we verify whether the entity embeddings are actually disentangled according to relations by our DisenE. In Figure 2(c), we visualize the attention values of a relation paying to $K$ components of different entities, where the y-coordinate is randomly sampled entities that appear in the same triplets with the relation. The heat map indicates that the same relation tends to focus on the same components.
Table 2: Link prediction results on WN18RR and FB15k-237. The best score is in bold and second best score is underlined. DisenE (TransE) and DisenE (ConvKB) indicate using TransE and ConvKB as feature extraction method for DisenE respectively. Results of [•] and [⋆] are taken from (Nguyen et al., 2018) and (Dettmers et al., 2018) respectively; Results of [◦] are reproduced according to original paper (Nathani et al., 2019). Other results are taken from the corresponding papers.

Figure 2: Figure (a) is t-SNE plots of learned relation attention value, where different colors indicate different focused components. Figure (b) is sensitivity experiments of $K$. Figure (c) and Figure (d) are relation and entity cases respectively, where the full names of them are listed in Appendix C.

of different entities. By analyzing the distribution of attention, we find that the relations that are mostly focus on the first component are generally related to sports events, which leads to the “gender” relation also focuses on the first component of male entities.

Moreover, to verify the learned representation satisfies the intuition that different relations focus on different components of entities, we plot the attention values on the components of the entity Britain in Figure 2(d), where the y-coordinate is sampled relations that appear in the same triplets with “Britain”. We observe that semantically similar relations have similar attention value distributions. For example, relations “gdp_nominal”, “gdp_real”, “dated_money”, “ppp_dollars”, are all related to economics, relations “olympic_medal”, “olympics”, “medal_won” are all related to Olympics competitions. These results demonstrate that the disentangled representations learned by our DisenE have certain interpretability. More detailed cases are presented in Appendix D.

5 Conclusion

We propose DisenE, an end-to-end framework that learns disentangled knowledge graph embeddings. Experimental results prove the effectiveness of our DisenE on link prediction task. Furthermore, our detailed analysis highlights the interpretable superiority of our proposed framework.

Acknowledgments

This work is supported by NSFC under Grant No. 61532001, National Key Research and Development Program of China under Grant No. 2018AAA0101902, MOE-ChinaMobile Program under Grant No. MCM20170503, and Big Education Data Research Program of Peking University under Grant No. 2020YBC13.
References

Alexander A Alemi, Ian Fischer, Joshua V Dillon, and Kevin Murphy. 2017. Deep variational information bottleneck. Proceedings of the International Conference on Learning Representations.

Ivana Balazevic, Carl Allen, and Timothy 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), pages 5188–5197.

Antoine Bordes, Nicolas Usunier, Alberto Garcia-Duran, Jason Weston, and Oksana Yakhanenko. 2013. Translating embeddings for modeling multi-relational data. In Advances in neural information processing systems, pages 2787–2795.

Antoine Bordes, Jason Weston, and Nicolas Usunier. 2014. Open question answering with weakly supervised embedding models. In Joint European Conference on Machine Learning and Knowledge Discovery in Databases, pages 165–180. Springer.

Tim Dettmers, Pasquale Minervini, Pontus Stenetorp, and Sebastian Riedel. 2018. Convolutional 2d knowledge graph embeddings. In Thirty-Second AAAI Conference on Artificial Intelligence.

Irina Higgins, Loic Matthey, Arka Pal, Christopher Burgess, Xavier Glorot, Matthew Botvinick, Shakir Mohamed, and Alexander Lerchner. 2017. beta-vae: Learning basic visual concepts with a constrained variational framework. Proceedings of the International Conference on Learning Representations, 2(5):6.

Shaoxiong Ji, Shirui Pan, Erik Cambria, Pekka Marttinen, and Philip S Yu. 2020. A survey on knowledge graphs: Representation, acquisition and applications. In the Association for the Advance of Artificial Intelligence Conference.

Seyed Mehran Kazemi and David Poole. 2018. Simple embedding for link prediction in knowledge graphs. In Advances in neural information processing systems.

Diederik P Kingma and Jimmy Ba. 2014. Adam: A method for stochastic optimization. arXiv preprint arXiv:1412.6980.

Yankai Lin, Zhiyuan Liu, Maosong Sun, Yang Liu, and Xuan Zhu. 2015. Learning entity and relation embeddings for knowledge graph completion. In Twenty-ninth AAAI conference on artificial intelligence.

Zachary C Lipton. 2018. The mythos of model interpretability. Queue, 16(3):31–57.

Laurens van der Maaten and Geoffrey Hinton. 2008. Visualizing data using t-sne. Journal of machine learning research, 9(Nov):2579–2605.

Deepak Nathani, Jatin Chauhan, Charu Sharma, and Manohar Kaul. 2019. Learning attention-based embeddings for relation prediction in knowledge graphs. In Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics, pages 4710–4723.

Dai Quoc Nguyen, Tu Dinh Nguyen, Dat Quoc Nguyen, and Dinh Phung. 2018. A novel embedding model for knowledge base completion based on convolutional neural network. In Proceedings of the 2018 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 2 (Short Papers), pages 327–333, New Orleans, Louisiana, June.

Kristina Toutanova and Danqi Chen. 2015. Observed versus latent features for knowledge base and text inference. In Proceedings of the 3rd Workshop on Continuous Vector Space Models and their Compositionality, pages 57–66.

Théo Trouillon, Johannes Welbl, Sebastian Riedel, Éric Gaussier, and Guillaume Bouchard. 2016. Complex embeddings for simple link prediction. In International Conference on Machine Learning, pages 2071–2080.

Zhen Wang, Jianwen Zhang, Jianlin Feng, and Zheng Chen. 2014. Knowledge graph embedding by translating on hyperplanes. In Twenty-Eighth AAAI conference on artificial intelligence.

Bishan Yang, Wen-tau Yih, Xiaodong He, Jianfeng Gao, and Li Deng. 2014. Embedding entities and relations for learning and inference in knowledge bases. arXiv preprint arXiv:1412.6575.
A Sensitivity Study

In this section, we investigate the sensitivity of the number of components $K$ under different experimental methods on the WN18RR dataset. From Figure 3, we find that our DisenE(TransE) method can get the highest MRR and lowest MR when $K = 2$, and DisenE(ConvKB) method achieve the best performance when $K = 4$. The reason is that WN18RR has a small number of relations and does not need to be disentangled into too many components.

![Figure 3: Parameter sensitivity of $K$ on WN18RR dataset.](image)

B Ablation Study

| Ablation                      | MRR | H@1 | H@10 |
|-------------------------------|-----|-----|------|
| Full DisenE(ConvKB)           | .478| .403| .626 |
| (-) Attention operation       | .451| .382| .591 |
| (-) Convolution operation     | .312| .225| .461 |
| (-) Additional Loss $L_{REL_1}$| .458| .361| .612 |
| (-) Additional Loss $L_{REL_2}$| .461| .363| .609 |

Table 3: Ablation study on FB15k-237 dataset by DisenE(ConvKB). “(-)” denotes without this operation.

Table 3 shows the results of the ablation study on the test set of FB15k-237 by DisenE(ConvKB) method. Removing attention operation can be seen as when the number of components $K = 1$, which means the model does not distinguish entity’s components. By removing convolution operation, the local correlation of the triplet would be omitted, thus the experimental results seriously affected. Moreover, the performance drop of removing additional loss $L_{REL_1}$ or $L_{REL_2}$ indicates it is a crucial component in DisenE, which can potentially handle the regularization of our model during the training process.

C Full Names

The full names of the entities and relations used in the main paper are shown in Table 4 and Table 5:

| Abbreviations | Id     | Descriptions                                      |
|---------------|--------|---------------------------------------------------|
| Henry         | /m/0fjy9| Henry John Deutschendorf                          |
| Alan          | /m/012wg| Alan Jay Lerner                                    |
| George        | /m/02qsjt| George BuddyGuy                                   |
| Anna          | /m/01pcq3| Anna Helene Paquin                                |
| Frank         | /m/02p7xc| Frank Skinner                                     |
| Daniel        | /m/068g3p| Daniel James Roebuck                              |
| Alan          | /m/02w29z| Alan Wray Tudyk                                   |
| Jesse         | /m/01nrq5| Jesse Donald                                      |
| Britain       | /m/07ssc| The United Kingdom of Great Britain and Northern Ireland |

Table 4: Specific names of entities in Section 3.5.

D More Cases

We provide more heat maps of attention values in Figure 4 and Fig. 5.
| Abbreviations | Specific relation names |
|--------------|------------------------|
| gender       | /people/person/gender   |
| member       | /organization/organization_member/member_of/organization/organization_membership/organization |
| founder      | /organization/organization_founder/organizations_founded |
| ppp_dollars  | /location/statistical_region/gni_per_capita_in_ppp_dollars/measurement_unit/dated_money_value/currency |
| measurement  | /location/statistical_region/gdp_nominal/measurement_unit/dated_money_value/currency |
| adjusted_money | /location/statistical_region/gdp_real/measurement_unit/adjusted_money_value/adjustment_currency |
| dated_money  | /location/statistical_region/gdp_nominal_per_capita/measurement_unit/dated_money_value/currency |
| athletes     | /olympics/olympic_participating_country/athletes/olympics/olympic_medal_honor/medal |
| olympics     | /olympics/olympic_participating_country/medals_won/olympics/olympic_medal_honor/medal |
| schema       | /base/aareas/schema/administrative_area/administrative_area_type |

Table 5: Specific names of relations in Section 3.5.

Figure 4: Cases trained on FB15k-237 using $K = 4$ and relation embedding size $l = 100$, which indicate that the same relation tends to focus on the same components of different entities. Noting that y-coordinate is the ids of entities.

Figure 5: Cases trained on FB15k-237 using $K = 4$ and relation embedding size $l = 100$, which indicate different relations focus on different components of the entities and the relations that have similar attention value distributions usually can gather a group. Noting that y-coordinate is the ids of relations.