InterHT: Knowledge Graph Embeddings by Interaction between Head and Tail Entities

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Abstract

Knowledge graph embedding (KGE) models learn the representation of entities and relations in knowledge graphs. Distance-based methods show promising performance on link prediction task, which predicts the result by the distance between two entity representations. However, most of these methods represent the head entity and tail entity separately, which limits the model capacity. We propose a novel distance-based method named InterHT that allows the head and tail entities to interact better and get better entity representation. Experimental results show that our proposed method achieves the best results on ogbl-wikikg2 dataset.

1 Introduction

Knowledge graph embedding (KGE) models learn the representation of entities and relations in the knowledge graphs (KGs). A large number of KGE methods have been proposed to solve the problem of knowledge graph completion. KGE can also be applied to various applications such as recommender systems, question answering and query expansion.

Nowadays, KGE methods have been widely studied. One of the most popular methods for KGE is the distance-based methods, such as transE (Bordes et al., 2013), transH (Wang et al., 2014), RotatE (Sun et al., 2019) and PairRE (Chao et al., 2020). These methods represent head and tail entities as deterministic vectors separately. This static entity representation limits the learning capacity of models, which prohibits models to better learn large-scale KG.

In natural language understanding tasks, the contextual representation of words is usually important for the downstream tasks. Inspired by this, we propose a novel distance-based method called InterHT which can represent the head and tail entities by combining the information of the tail and head entities, respectively. Concretely, for the head entity embedding, we element-wise multiply the original head entity representation with an auxiliary tail entity vector to obtain the final representation of the head entity. By this way, we can incorporate the information of the tail entity into the head entity representation. Similarly, we can use the same method to obtain the final representation of the tail entity.

We validate our model on the ogbl-wikikg2 dataset (Hu et al., 2020). The InterHT achieve 67.79\% in MRR, which yields a 1.97\% increment over the state-of-the-art model. The experimental results show that our proposed approach effectively improves the model capacity and achieves the best performance on the dataset.

2 Related Work

The link prediction task on KGs is conventionally accomplished via KGE approaches. Generally, these approaches can be categorised into two families, distance-base models and bilinear models. Distance-based models represent the fact \((h, r, t)\) in embedding spaces and measure the distance between entities. Usually, they approximate the tail entity vector \(t\) via translating the head entity vector \(h\) by the relation vector \(r\), and measure the distance between this translated entity and the actual tail entity. The closer distance indicates the higher plausibility that the fact \((h, r, t)\) holds. TransX series models, such as TransE/H/R/D (Bordes et al., 2013; Wang et al., 2014; Lin et al., 2015; Ji et al., 2015), manipulate in the real space. Among the series, TransE represents entities and relations in a single space for 1to1 mapping. Its extensions employ hyperplane (TransH) and multiple embedding spaces (TransR, TranD, etc) to handle complex relations. RotatE(Sun et al., 2019) introduces the rotation translation in complex space for modeling more complicated relation patterns.

To gain better expressiveness, researchers further exploit high dimension spaces, directed rela-
sions and multiple relation vectors. For example, GC-OTE(Tang et al., 2019) performs orthogonal transformation and enriches the representation with directed relation vectors, and PairRe(Chao et al., 2020) uses two vectors to represent a single relation. While entity and relation vectors in these embedding spaces are expressed as deterministic vectors, some methods (TransG(Xiao et al., 2015), etc.) emphasize the uncertainty of nodes and links via Gaussian distribution. The amount of parameters of the above models grow markedly along with the improvement of performance, yet they could still suffer from out-of-vocabulary (OOV) problem. NodePiece(Galkin et al., 2021) proposes to tokenise entity nodes into sets of anchors which dramatically reduces the parameter size and provides better generalization to unseen entities.

Instead of measuring the distance, bilinear models scoring the candidates by semantic similarity. RESCAL(Nickel et al., 2011), TATEC(García-Durán et al., 2014), DisMult(Yang et al., 2014) and HolE(Nickel et al., 2016) represent entities in real space, and interact head and tail entities according to matrix decomposition to learn the relation matrix. ComplEx(Trouillon et al., 2016) extends the embedding space to complex domain to take advantage of the Hermitian dot product. Since Hermitian product is not commutative, it helps to better capture asymmetric relations. Other approaches measure the similarity directly through deep neural networks and graph neural networks, for instance, SME(Bordes et al., 2014), NAM(Liu et al., 2016), GNNs(Li et al., 2016; Gilmer et al., 2017; Xu et al., 2019), etc.

Apart from the commonly used distance-based models and bilinear models, automated machine learning methods, pretrained language models and some retrieval-reranking methods are also used in KG completion tasks. For instance, AutoSF(Zhang et al., 2020) manages to design and search for better data-dependant scoring functions automatically; KG-BERT(Yao et al., 2019) treats the fact triples as text sequences and converts KG completion tasks into classification tasks; Cao et al. (2021) discuss and compare several prompt-based pre-training methods on KGS; Lovelace et al. (2021) propose a robust KG completion method with a student re-ranking network.

3 Method

In previous research, both head and tail entities are represented independently. We proposed a novel distance-based method named InterHT. The InterHT incorporate the information of the tail entity into the head entity representation, which can improve the model capacity.

3.1 InterHT

The illustration of the proposed InterHT is shown in Figure 1. The final embedding of an entity is generated by interacting over an auxiliary representation of the other entity in the same fact. For the head entity embedding, we element-wise multiply the original head entity representation with an auxiliary tail entity vector to obtain the final representation of the head entity. Similarly, we can use the same method to obtain the final representation of the tail entity. The equations are as follows:

\[
|h \circ t_a - t \circ h_a + r| \quad (1)
\]

where \(t_a\) is auxiliary tail entity vector and \(h_a\) is auxiliary tail entity vector. Similar to Yu et al. (2021), we add a unit vector \(e\) to \(t_a\) and \(h_a\).

\[
|h \circ (t_a + e) - t \circ (h_a + e) + r| \quad (2)
\]

\(h \circ (t_a + e)\) is the representation of the head that combines information of the tail, and \(t \circ (h_a + e)\) is the representation of the tail integrating information of the head. We also use the NodePiece to learn a fixed-size entity vocabulary, which can alleviate the OOV problem.

3.2 Loss Function

To optimize the model, we utilize the self-adversarial negative sampling loss as the loss function for training (Sun et al., 2019). The loss function is as follows:

\[
L = -\log \sigma(\gamma - d_r(h, t))
- \sum_{i=1}^{n} \frac{1}{k} \log \sigma(d_r(h_i, t_i') - \gamma) \quad (3)
\]

where \(\gamma\) is a fixed margin, \(\sigma\) is the sigmoid function, and \((h_i', r, t_i')\) is the \(i\)-th negative triplet.

4 Experiments

4.1 Experimental Setup

Dataset In this paper we use the ogbl-wikikg2 dataset to validate our approach. ogbl-wikikg2
is extracted from Wikidata knowledge base. One of the main challenges for this dataset is complex relations. The statistics of the dataset are shown in Table 1. The MRR metric is adopted for evaluation.

### Baseline Models
For a sufficient comparison, we employ several typical models for the KG completion tasks and some well-performed combined methods as baselines, including distance-based models, bilinear models and some enhancing approaches. Baseline models include TransE, RotatE, PairRE, TripleRE, DisMult, ComplEx and AutoSF. Enhancing approaches include NodePiece and Relation prediction (RP)(Chen et al., 2021). RP refers to the relation type prediction task, which predicts the relation type given the head and tail entities of a fact. We give a brief demonstration of each method here:

- **TransE** (Bordes et al., 2013) represents the fact \((h, r, t)\) as vectors, the head entity vector \(h\) is translated by relation vector \(r\) and the target is to approximate the tail entity vector \(t\), i.e., \(h + r \approx t\). The scoring function is \(-\|h + r - t\|\).

- **RotatE** (Sun et al., 2019) rotates the head entity vector by the relation vector on a unit circle, i.e., \(h \circ r = t\). The scoring function is \(-\|h \circ r - t\|\).

- **PairRE** (Chao et al., 2020) represents the relation with two vectors, \(r^H\) and \(r^T\), to encode complex relation and multiple relation patterns. The corresponding scoring function is \(-\|h \circ r^H - h \circ r^T\|\).

- **TripleRE** (Yu et al., 2021) adds a relation translation to the scoring function of PairRE and proposes two versions of scoring function. We refer to the first version (TripleREv1) for TripleRE baseline, which is as follow, \(-\|h \circ r^h - h \circ r^t + r^m\|\). The other is called TripleREv2 and is used in TripleRE+NodePiece baseline, specific, \(-\|h \circ (r^h + u \ast e) - h \circ (r^t + u \ast e) + r^m\|\), where \(u\) is a constant and \(e\) is a unit vector.

- **DisMult** (Yang et al., 2014) relation matrix \(M_r\) is restricted to a diagnose matrix and models only the symmetric relations. The scoring function is \(h^\top diag(r) t\).

- **ComplEx** (Trouillon et al., 2016) represents nodes in complex space and scores the real part of the relation matrix, i.e., \(RE(h^\top diag(r) \bar{t})\), where \(\bar{t}\) is the complex conjugate of the tail vector \(t\).

- **AutoSF** (Zhang et al., 2020) is a two-stage approach to automatically design a best data-dependent scoring function. It first learns a set of the converged model parameters on the training set, and then search for a better scoring scheme on the validation set.

- **AutoSF+NodePiece** embeds entities with respect to the anchor-based approach and uses AutoSF to design the scoring function.

- **TripleRE+NodePiece** used NodePiece entity embeddings and TripleREv2 scoring function.

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Table 1: Dataset statistics. LP means link prediction.

| Dataset   | Task | Nodes | Relations | Edges   | Train   | Validation | Test    |
|-----------|------|-------|-----------|---------|---------|------------|---------|
| OGB WikiKG2 | LP   | 2,500,604 | 535       | 17,137,181 | 16,109,182 | 429,456   | 598,543 |

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Figure 1: Illustration of InterHT.
| Model                  | #Params | Test MRR         | Valid MRR        |
|-----------------------|---------|------------------|------------------|
| TransE (500dim)       | 1251M   | 0.4256 ± 0.0030  | 0.4272 ± 0.0030  |
| RotatE (250dim)       | 1250M   | 0.4332 ± 0.0025  | 0.4353 ± 0.0028  |
| PairRE (200dim)       | 500M    | 0.5208 ± 0.0027  | 0.5423 ± 0.0020  |
| AutoSF                | 500M    | 0.5458 ± 0.0052  | 0.5510 ± 0.0063  |
| ComplEx (250dim)      | 1251M   | 0.5027 ± 0.0027  | 0.3759 ± 0.0016  |
| TripleRE              | 501M    | 0.5794 ± 0.0020  | 0.6045 ± 0.0024  |
| ComplEx-RP (50dim)    | 250M    | 0.6392 ± 0.0045  | 0.6561 ± 0.0070  |
| AutoSF + NodePiece    | 6.9M    | 0.5703 ± 0.0035  | 0.5806 ± 0.0047  |
| TripleRE + NodePiece  | 7.3M    | 0.6582 ± 0.0020  | 0.6616 ± 0.0018  |
| InterHT + NodePiece   | 19.2M   | 0.6779 ± 0.0018  | 0.6893 ± 0.0015  |

Table 2: Experimental results.

- ComplEx-RP adds the relation prediction probability, $\lambda log P_{\theta}(r|h,t)$, to ComplEx’s training objective.

**Model Hyperparameters** We utilize Adam optimizer with learning rate of 5e-4. The training batch size is set to 512. We set the maximum number of training steps to 500,000 and validate every 20,000 steps. The dimension of entity embedding is set to 200, and the negative sample size is 128. The number of anchors for NodePiece are 20,000.

### 4.2 Experimental Results

The experimental results are shown in Table 2. From the experimental results, we can see that InterHT achieves better performance than transE, which indicates that InterHT has a stronger model capacity. After adding NodePiece, InterHT achieves 67.79% in MRR, which yields a 1.97% increment over TripleRE. The experimental results show that our proposed approach effectively improves the model capacity and achieves the best results on ogbl-wikikg2 dataset.

### 4.3 Conclusion

In this paper, we propose a novel distance-based knowledge graph embedding model named InterHT. Our proposed method enhance the learning ability of the model with additional head and tail interactions. Experimental results show that our method achieves the best results on ogbl-wikikg2 dataset, reaching 67.79% in MRR on the test set.

### References

Antoine Bordes, Xavier Glorot, Jason Weston, and Yoshua Bengio. 2014. A semantic matching energy function for learning with multi-relational data. *Mach. Learn.*, 94(2):233–259.

Antoine Bordes, Nicolas Usunier, Alberto Garcia-Duran, Jason Weston, and Oksana Yakhnenko. 2013. Translating embeddings for modeling multi-relational data. *Advances in neural information processing systems*, 26.

Boxi Cao, Hongyu Lin, Xianpei Han, Le Sun, Lingyong Yan, Meng Liao, Tong Xue, and Jin Xu. 2021. Knowledgeable or educated guess? revisiting language models as knowledge bases. *In Proceedings of the 59th Annual Meeting of the Association for Computational Linguistics and the 11th International Joint Conference on Natural Language Processing (Volume 1: Long Papers)*, pages 1860–1874, Online. Association for Computational Linguistics.

Linlin Chao, Jiashan He, Taifeng Wang, and Wei Chu. 2020. Paire: Knowledge graph embeddings via paired relation vectors. *arXiv preprint arXiv:2011.03798*.

Yihong Chen, Pasquale Minervini, Sebastian Riedel, and Pontus Stenetorp. 2021. Relation prediction as an auxiliary training objective for improving multi-relational graph representations. *In 3rd Conference on Automated Knowledge Base Construction*.

Mikhail Galkin, Jiapeng Wu, Etienne Denis, and William L Hamilton. 2021. Nodepiece: Compositional and parameter-efficient representations of large knowledge graphs. *arXiv preprint arXiv:2106.12144*.

Alberto García-Durán, Antoine Bordes, and Nicolas Usunier. 2014. Effective blending of two and three-way interactions for modeling multi-relational data. *In Proceedings of the 2014th European Conference on Machine Learning and Knowledge Discovery in Databases - Volume Part I, ECMLPKDD’14*, page 434–449, Berlin, Heidelberg. Springer-Verlag.
Justin Gilmer, Samuel S. Schoenholz, Patrick F. Riley, Oriol Vinyals, and George E. Dahl. 2017. Neuronal message passing for quantum chemistry. In Proceedings of the 34th International Conference on Machine Learning - Volume 70, ICML'17, page 1263–1272. JMLR.org.

Weihua Hu, Matthias Fey, Marinka Zitnik, Yuxiao Dong, Hongyu Ren, Bowen Liu, Michele Catasta, and Jure Leskovec. 2020. Open graph benchmark: Datasets for machine learning on graphs. Advances in neural information processing systems, 33:22118–22133.

Guoliang Ji, Shizhu He, Liheng Xu, Kang Liu, and Jun Zhao. 2015. Knowledge graph embedding via dynamic mapping matrix. In Proceedings of the 53rd annual meeting of the association for computational linguistics and the 7th international joint conference on natural language processing (volume 1: Long papers), pages 687–696.

Yujia Li, Richard Zemel, Marc Brockschmidt, and Daniel Tarlow. 2016. Gated graph sequence neural networks. In Proceedings of ICLR’16.

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.

Quan Liu, Hui Jiang, Zhen-Hua Ling, Si Wei, and Yu Hu. 2016. Probabilistic reasoning via deep learning: Neural association models. CoRR, abs/1603.07704.

Justin Lovelace, Denis Newman-Griffis, Shikhar Vashisht, Jill Fain Lehman, and Carolyn Rosé. 2021. Robust knowledge graph completion with stacked convolutions and a student re-ranking network. In Proceedings of the 59th Annual Meeting of the Association for Computational Linguistics and the 11th International Joint Conference on Natural Language Processing (Volume 1: Long Papers), pages 1016–1029, Online. Association for Computational Linguistics.

Maximilian Nickel, Lorenzo Rosasco, and Tomaso Poggio. 2016. Holographic embeddings of knowledge graphs. In Proceedings of the Thirtieth AAAI Conference on Artificial Intelligence, AAAI’16, page 1955–1961. AAAI Press.

Maximilian Nickel, Volker Tresp, and Hans-Peter Kriegel. 2011. A three-way model for collective learning on multi-relational data. In Proceedings of the 28th International Conference on International Conference on Machine Learning, ICML’11, page 809–816, Madison, WI, USA. Omnipress.

Zhiqing Sun, Zhi-Hong Deng, Jian-Yun Nie, and Jian Tang. 2019. Rotate: Knowledge graph embedding by rotational in complex space. arXiv preprint arXiv:1902.10197.

Yun Tang, Jing Huang, Guangtao Wang, Xiaodong He, and Bowen Zhou. 2019. Orthogonal relation transforms with graph context modeling for knowledge graph embedding. arXiv preprint arXiv:1911.04910.

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. PMLR.

Zhen Wang, Jianwen Zhang, Jianlin Feng, and Zheng Chen. 2014. Knowledge graph embedding by translating on hyperplanes. In Proceedings of the AAAI Conference on Artificial Intelligence, volume 28.

Han Xiao, Minlie Huang, Yu Hao, and Xiaoyan Zhu. 2015. TransG: A generative mixture model for knowledge graph embedding. arXiv preprint arXiv:1509.05488.

Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. 2019. How powerful are graph neural networks? In International Conference on Learning Representations.

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.

Liang Yao, Chengsheng Mao, and Yuan Luo. 2019. KG-BERT: BERT for knowledge graph completion. CoRR, abs/1909.03193.

Long Yu, ZhiCong Luo, Deng Lin, HuanYong Liu, and YaFeng Deng. 2021. Triplere: Knowledge graph embeddings via triple relation vectors. viXra preprint viXra:2112.0095.

Yongqi Zhang, Quanming Yao, Wenyuan Dai, and Lei Chen. 2020. Autosf: Searching scoring functions for knowledge graph embedding. In 2020 IEEE 36th International Conference on Data Engineering (ICDE), pages 433–444. IEEE.