Abstract

Knowledge Graph Completion (KGC) aims at automatically predicting missing links for large-scale knowledge graphs. A vast number of state-of-the-art KGC techniques have been published in top conferences in several research fields, including data mining, machine learning, and natural language processing. However, we notice that several recent papers report very high performance, which largely outperforms previous state-of-the-art methods. In this paper, we find that this can be attributed to the inappropriate evaluation protocol used by them and propose a simple evaluation protocol to address this problem. The proposed protocol is robust to handle bias in the model, which can substantially affect the final results. We conduct extensive experiments and report the performance of several existing methods using our protocol.

1 Introduction

Real-world knowledge bases are usually expressed as multi-relational graphs, which are collections of factual triplets, where each triplet \((h, r, t)\) represents a relation \(r\) between a head entity \(h\) and a tail entity \(t\). Examples of knowledge graphs include Freebase (Bollacker et al., 2008), YAGO (Suchanek et al., 2007), DBpedia (Lehmann et al., 2015), and WordNet (Miller, 1995). However, these real-word knowledge bases are usually incomplete (Dong et al., 2014), which motivates the research of automatically predicting missing links.

A popular approach for Knowledge Graph Completion (KGC) is to embed entities and relations into continuous vector or matrix space, and use a well-designed score function \(f(h, r, t)\) to measure the plausibility of the triplet \((h, r, t)\). Most of the previous methods use translation distance based (Bordes et al., 2013; Wang et al., 2014; Xiao et al., 2016; Sun et al., 2019) and semantic matching based (Nickel and Tresp, 2013; Yang et al., 2014; Nickel et al., 2016; Trouillon et al., 2016; Liu et al., 2017) scoring functions which are easy to analyze.

However, recently, a vast number of neural network-based methods have been proposed. They have complex score functions which utilize black-box neural networks including Convolutional Neural Networks (CNNs) (Dettmers et al., 2018; Nguyen et al., 2018), Recurrent Neural Networks (RNNs) (Lin et al., 2015; Wang et al., 2018), Graph Neural Networks (GNNs) (Schlichtkrull et al., 2017; Shang et al., 2019), and Capsule Networks (Nguyen et al., 2019). While some of them report state-of-the-art performance on several benchmark datasets that are competitive to previous embedding-based approaches, a considerable portion of recent neural network-based papers report very high performance gains which are not consistent across different datasets. Moreover, most of these unusual behaviors are not at all analyzed. Such a pattern has become prominent and is misleading the whole community.

In this paper, we investigate this problem and find that this is attributed to the inappropriate evaluation protocol used by these approaches. We demonstrate that their evaluation protocol gives a perfect score to a model that always outputs a constant irrespective of the input. This has lead to artificial inflation of performance of several models. For this, we find a simple evaluation protocol that creates a fair comparison environment for all types of score functions. We conduct extensive experiments to re-examine some recent methods and fairly compare them with existing approaches. Our contributions can be summarized as follows:

1. We highlight unusual behavior of some of the recently proposed Knowledge Graph Com-
pletion methods and demonstrate the bias in their evaluation protocol.

2. We find a simple evaluation protocol that creates a fair comparison environment for all types of score function.

3. We report the performance of several recent methods using our proposed protocol and fair comparison with prior approaches.

The source code and datasets used in the paper are available at http://github.com/svjan5/kgc-reevaluation.

2 Background and Related Work

Knowledge Graph Completion Given a Knowledge Graph $\mathcal{G} = (\mathcal{E}, \mathcal{R}, \mathcal{T})$, where $\mathcal{E}$ and $\mathcal{R}$ denote the set of entities and relations and $\mathcal{T} = \{(h, r, t) \mid h, t \in \mathcal{E}, r \in \mathcal{R}\}$ is the set of triplets (facts), the task of Knowledge Graph Completion (KGC) involves inferring missing facts based on the known facts. Most of the existing methods define an embedding for each entity and relation in $\mathcal{G}$, i.e., $e_h, e_r \forall h \in \mathcal{E}, r \in \mathcal{R}$ and a score function $f(h, r, t) : \mathcal{E} \times \mathcal{R} \times \mathcal{E} \rightarrow \mathbb{R}$ which assigns a high score for valid triplets than the invalid ones.

KGC Evaluation During KGC evaluation, for predicting $t$ in a given triplet $(h, r, t)$, a KGC model scores all the triplets in the set $\mathcal{T}^t = \{(h, r, t') \mid t' \in \mathcal{E}\}$. Based on the score, the model first sorts all the triplets and subsequently finds the rank of the valid triplet $(h, r, t)$ in the list. In a more relaxed setting called filtered setting, all the known correct triplets (from train, valid, and test triplets) are removed from $\mathcal{T}^t$ except the one being evaluated (Bordes et al., 2013). The triplets in $\mathcal{T}^t - \{t\}$ are called negative samples.

Existing Analysis of KGC Methods Prior to our work, Kadlec et al. (2017) cast doubt on the claim that performance improvement of several models is due to architectural changes as opposed to hyperparameter tuning or different training objective. In our work, we raise similar concerns but through a different angle by highlighting issues with the evaluation procedure used by several recent methods. Chandrasah et al. (2018) analyze the geometry of KG embeddings and its correlation with task performance while Nayyeri et al. (2019) examine the effect of different loss functions on performance. However, their analysis is restricted to non-neural approaches.

3 Observations

In this section, we first describe our observations and concerns and then investigate what leads to it.

3.1 Inconsistent Improvements over Benchmark Datasets

Several recently proposed methods report high performance gains on a particular dataset. However, their performance on another dataset is not consistently improved. In Table 1, we report change in MRR score on FB15k-237 (Toutanova and Chen, 2015) and WN18RR (Dettmers et al., 2018) datasets with respect to ConvE (Dettmers et al., 2018) for different methods including RotatE (Sun et al., 2019), TuckER (Balažević et al., 2019), ConvKB (Nguyen et al., 2018), CapsE (Nguyen et al., 2019), KBAT (Nathani et al., 2019), and TransGate (Yuan et al., 2019). Overall, we find that for a few recent NN based methods, there are inconsistent gains on these two datasets. For instance, in ConvKB, there is a 21.8% improvement over ConvE on FB15k-237, but a degradation of 42.3% on WN18RR, which is surprising given the method is claimed to be better than ConvE. On the other hand, methods like RotatE and TuckER give consistent improvement across both benchmark datasets.

|               | FB15k-237 | WN18RR |
|---------------|-----------|--------|
| ConvE         | .325      | .430   |
| RotatE        | .338 (+4.0%) | .476 (+10.6%) |
| TuckER        | .358 (+10.2%) | .470 (+9.3%) |
| ConvKB        | .396 (+21.8%) | .248 (-42.3%) |
| CapsE         | .523 (+60.9%) | .415 (-3.4%) |
| KBAT          | .518 (+59.4%) | .440 (+2.3%) |
| TransGate     | .404 (+24.3%) | .409 (-4.9%) |

Table 1: Changes in MRR for different methods on FB15k-237 and WN18RR datasets with respect to ConvE show inconsistent improvements. Overall, we find that non-NN based methods such as RotatE and TuckER give consistent improvement over both datasets whereas for some NN based methods the performance improves on one dataset while degrades on another. Refer to Section 3.1 for details.
3.2 Observations on Score Functions

Score distribution When evaluating KGC methods, for a given triplet $(h, r, t)$, the ranking of $t$ given $h$ and $r$ is computed by scoring all the triplets of form \{$(h, r, t') : t' \in \mathcal{E}$\}. On investing a few recent NN based approaches, we find that they have unusual score distribution, where some negatively sampled triplets have the same score as the valid triplet. An instance of FB15k-237 dataset is presented in Figure 1. Here, out of 14,541 negatively sampled triplets, 8,520 have the exact same score as the valid triplet.

Statistics on the whole dataset In Figure 2, we report the total number of triplets with the exact same score over the entire dataset for ConvKB (Nguyen et al., 2018) and CapsE (Nguyen et al., 2019) and compare them with ConvE (Dettmers et al., 2018) which does not suffer from this issue. We find that both ConvKB and CapsE have multiple occurrences of such unusual score distribution. On average, ConvKB and CapsE have 125 and 278 entities with exactly same score as the valid triplet over the entire evaluation dataset of FB15k-237, whereas ConvE has around 0.002, which is almost negligible. In Section 4, we demonstrate how this leads to massive performance gain for methods like ConvKB and CapsE.

Root of the problem Further, we investigate the cause behind such unusual score distribution. In Figure 3, we plot the ratio of neurons becoming zero after ReLU activation for the valid triplets vs. their normalized frequency on FB15k-237 dataset. The results show that in ConvKB and CapsE, a large fraction (87.3% and 92.2% respectively) of the neurons become zeros after applying ReLU activation. However, with ConvE, this count is substantially less (around 41.1%). Because of the zeroing of nearly all neurons (at least 14.2% for ConvKB and 22.0% for CapsE), the representation of several triplets become very similar during forward pass and thus leading to obtaining the exact same score.

4 Evaluation Method

In this section, we present different evaluation methodologies that can be adopted in knowledge graph completion. We further show that inappropriate evaluation protocol is the key reason for the unusual behavior of some recent NN based methods.

How to deal with the same scores? An essential aspect of the evaluation method is to decide how to break ties for triplets with the same score. More concretely, while scoring $\mathcal{T}'$, if there are multiple triplets with the same score from the model, one should decide which triplet to pick. Based on this choice, we design a general evaluation scheme for KGC, which consists of following three different protocols in which the correct triplet $(h, r, t)$ can be placed in $\mathcal{T}'$:

1. **TOP**: In this setting, the correct triplet is inserted in the beginning of $\mathcal{T}'$. 
Figure 3: Distribution of ratio of neurons becoming zero after ReLU activation in different methods for the valid triplets in FB15k-237 dataset. We find that for ConvKB and CapsE an unusually large fraction of neurons become zero after ReLU activation whereas the does not hold with ConvE. More details presented in Section 3.2.

2. **BOTTOM**: Here, the correct triplet is inserted at the end of \( \mathcal{T}^\prime \).

3. **RANDOM**: In this, the correct triplet is placed randomly in \( \mathcal{T}^\prime \).

We assume that the triplets are sorted in a stable manner, i.e., the relative order of triplets with equal scores is maintained while sorting. Based on the definition of the three evaluation protocols, we have the following proposition.

**Proposition 4.1.** A score function that gives a constant score to all triplets irrespective of the input, i.e., \( f(h, r, t) = c \), achieves the best performance when evaluated using TOP evaluation scheme.

From Proposition 4.1, it is clear that TOP evaluation protocol does not evaluate the model rigorously. It gives the models that have a bias to provide the same score for different triplets, an inappropriate advantage. On the other hand, BOTTOM evaluation protocol can be unfair to the model during inference time because it penalizes the model for giving the same score to multiple triplets, i.e., if many triplets have the same score as the correct triple, the correct triplet gets the least rank possible.

As a result, RANDOM is the best evaluation technique which is both rigorous and fair to the model. It is in line with the situation we meet in the real world: given several same scored candidates, the only option is to select one of them randomly. Hence, we propose to use RANDOM evaluation scheme for all model performance comparisons.

## 5 Experiments

In this section, we conduct extensive experiments using our proposed evaluation protocols and make a fair comparison for several existing methods.

### 5.1 Datasets

We use two common benchmark datasets described below:

- **FB15k-237** (Toutanova and Chen, 2015) is a subset of FB15k (Bordes et al., 2013) with inverse relations deleted to prevent direct inference of test triples from training.
- **WN18RR** (Dettmers et al., 2018) is a subset of WN18 (Bordes et al., 2013) containing lexical relations between words. Similar to FB15k-237, inverse relations are removed in WN18RR.

### 5.2 Methods Analyzed

In our experiments, we categorize methods into the following two categories.

- **Non-Affected**: This includes methods which give consistent performance under different evaluation protocols. For experiments in this paper, we consider three such methods – ConvE (Dettmers et al., 2018), RotatE (Sun et al., 2019), and TuckER (Balažević et al., 2019).
- **Affected**: This category consists of recently proposed neural-network based methods whose performance is affected by different evaluation protocols. ConvKB (Nguyen et al., 2018), CapsE (Nguyen et al., 2019), TransGate (Yuan et al., 2019), and KBAT (Nathani et al., 2019) are methods in this category.

### 5.3 Evaluation Metrics

For all the methods, we use the code and the hyper-parameters provided by the authors in their respective papers. Model performance is evaluated using three standard metrics - Mean Reciprocal Rank (MRR), Mean Rank (MR) and Hits@10 (H@10) on filtered setting (Bordes et al., 2013).

### 5.4 Evaluation Results

To analyze the effect of different evaluation protocols described in Section 4, we study the performance variation of the models listed in Section
5.2. We study the effect of using **TOP** and **BOTTOM** protocols and compare them to the **RANDOM** protocol. We also study the random error in **RANDOM** protocol with multiple runs, where we report the average and standard deviation on 5 runs with different random seeds.

The results on FB15k-237 and WN18RR are presented in Tables 2 and 3, respectively. In their original paper, ConvE, RotatE, and TuckER use a strategy similar to the proposed **RANDOM** protocol, while ConvKB, CapsE, and KBAT use **TOP** protocol. We observe that for Non-Affected methods like ConvE, RotatE, and TuckER, the performance remains consistent across different evaluation protocols. However, with Affected methods, there is a considerable variation in performance. Specifically, we can observe that these models perform best when evaluated using **TOP** and worst when evaluated using **BOTTOM**. Finally, we find that the proposed **RANDOM** protocol is very robust to different random seeds. Although the theoretical upper and lower bounds of a **RANDOM** score are **TOP** and **BOTTOM** scores respectively, when we evaluate knowledge graph completion for real-world large-scale knowledge graphs, the randomness won’t affect the evaluation results much.

### 6 Conclusion

In this paper, we performed an extensive re-examination study of recent neural network based KGC techniques that claim very high performance on certain datasets. We find that many such models have issues with their score functions. **KBAT** incorporates ConvKB in the last layer of its model architecture, which should be affected by different evaluation protocols. But we find another bug on the leakage of test triples during negative sampling in the reported model, which results in more significant performance degradation.

---

**Table 2:** Effect of different evaluation protocols on recent KG embedding methods on FB15k-237 dataset. For **TOP** and **BOTTOM**, we report changes in performance with respect to **RANDOM** protocol. Please refer to Section 5.4 for details. †: KBAT has test data leakage in their original implementation.

|      | **Reported** | **RANDOM** | **TOP** | **BOTTOM** |
|------|--------------|------------|---------|------------|
|      | MRR | MR | H@10 | MRR | MR | H@10 | MRR | MR | H@10 |
| ConvE | .325 | 244 | .501 | .324 | 285 | .501 | .324 | 285 | .501 |
| RotatE | .338 | 177 | .533 | .336 | 178 | .530 | .336 | 178 | .530 |
| TuckER | .358 | - | .544 | .353 | 162 | .536 | .353 | 162 | .536 |
| ConvKB | .396 | 257 | .517 | .407 | 246 | .527 | .130 | 270 | .331 |
| CapsE | .523 | 303 | .593 | .511 | 305 | .586 | .009 | 585 | .000 |
| KBAT | .518† | 210† | .626† | .511 | 210† | .626† | .511 | 210† | .626† |

|      | **Reported** | **RANDOM** | **TOP** | **BOTTOM** |
|------|--------------|------------|---------|------------|
|      | MRR | MR | H@10 | MRR | MR | H@10 | MRR | MR | H@10 |
| ConvE | .43 | 4187 | .52 | .444 | 4950 | .503 | .444 | 4950 | .503 |
| RotatE | .476 | 3340 | .571 | .473 | 3343 | .571 | .473 | 3343 | .571 |
| TuckER | .470 | - | .526 | .461 | 6324 | .516 | .461 | 6324 | .516 |
| ConvKB | .248 | 2554 | .525 | .251 | 1696 | .516 | .164 | 6324 | .516 |
| CapsE‡ | .415 | 719 | .560 | .415 | 718 | .559 | .030 | 585 | .000 |
| KBAT | .440‡ | 1940‡ | .581‡ | .412 | 1921 | .554 | .412 | 1921 | .554 |

**Table 3:** Performance comparison under different evaluation protocols on WN18RR dataset. For **TOP** and **BOTTOM**, we report changes in performance with respect to **RANDOM** protocol. Please refer to Section 5.4 for details. †: KBAT has test data leakage in their original implementation. ‡: CapsE uses the pre-trained 100-dimensional Glove (Pennington et al., 2014) word embeddings for initialization on WN18RR dataset, which makes the comparison on WN18RR still unfair. †: KBAT has test data leakage in their original implementation.
bined with inappropriate evaluation protocol, such methods reported inflated performance. Based on our observations, we propose RANDOM evaluation protocol that can clearly distinguish between these affected methods from others. We also strongly encourage the research community to follow the RANDOM evaluation protocol for all KGC evaluation purposes.

References

Ivana Balažević, Carl Allen, and Timothy M Hospedales. 2019. Tucker: Tensor factorization for knowledge graph completion. In Empirical Methods in Natural Language Processing.

Kurt Bollacker, Colin Evans, Praveen Paritosh, Tim Sturge, and Jamie Taylor. 2008. Freebase: A collaboratively created graph database for structuring human knowledge. In Proceedings of the 2008 ACM SIGMOD International Conference on Management of Data, SIGMOD ’08, pages 1247–1250, New York, NY, USA. ACM.

Antoine Bordes, Nicolas Usunier, Alberto Garcia-Duran, Jason Weston, and Oksana Yakhnenko. 2013. Translating embeddings for modeling multi-relational data. In C. J. C. Burges, L. Bottou, M. Welling, Z. Ghahramani, and K. Q. Weinberger, editors, Advances in Neural Information Processing Systems 26, pages 2787–2795. Curran Associates, Inc.

Chandrasah, Aditya Sharma, and Partha Talukdar. 2018. Towards understanding the geometry of knowledge graph embeddings. In Proceedings of the 56th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), pages 122–131, Melbourne, Australia. Association for Computational Linguistics.

Tim Dettmers, Minervini Pasquale, Stenetorp Pontus, and Sebastian Riedel. 2018. Convolutional 2d knowledge graph embeddings. In Proceedings of the 32th AAAI Conference on Artificial Intelligence, pages 1811–1818.

Xin Dong, Evgeniy Gabrilovich, Geremy Heitz, Wilko Horn, Ni Lao, Kevin Murphy, Thomas Strohmann, Shaohua Sun, and Wei Zhang. 2014. Knowledge vault: A web-scale approach to probabilistic knowledge fusion. In Proceedings of the 20th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, KDD ’14, pages 601–610, New York, NY, USA. ACM.

Rudolf Kadlec, Ondrej Bajgar, and Jan Kleindienst. 2017. Knowledge base completion: Baselines strike back. In Proceedings of the 2nd Workshop on Representation Learning for NLP, pages 69–74, Vancouver, Canada. Association for Computational Linguistics.

Jens Lehmann, Robert Isele, Max Jakob, Anja Jentsch, Dimitris Kontokostas, Pablo N. Mendes, Sebastian Hellmann, Mohamed Morsey, Patrick van Kleef, Sören Auer, and Christian Bizer. 2015. Dbpedia - a large-scale, multilingual knowledge base extracted from wikipedia. Semantic Web, 6:167–195.

Yankai Lin, Zhiyuan Liu, Huanbo Luan, Maosong Sun, Siwei Rao, and Song Liu. 2015. Modeling relation paths for representation learning of knowledge bases. In Proceedings of the 2015 Conference on Empirical Methods in Natural Language Processing, pages 705–714, Lisbon, Portugal. Association for Computational Linguistics.

Hanxiao Liu, Yuxin Wu, and Yiming Yang. 2017. Analogical inference for multi-relational embeddings. In Proceedings of the 34th International Conference on Machine Learning, volume 70 of Proceedings of Machine Learning Research, pages 2168–2178, International Convention Centre, Sydney, Australia. PMLR.

George A. Miller. 1995. Wordnet: A lexical database for english. Commun. ACM, 38(11):39–41.

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. Association for Computational Linguistics.

Mojtaba Nayyeri, Chengjin Xu, Yadollah Yaghoobzadeh, Hamed Shariat Yazdi, and Jens Lehmann. 2019. Toward Understanding The Effect Of Loss function On Then Performance Of Knowledge Graph Embedding. arXiv e-prints, page arXiv:1909.00519.

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. Association for Computational Linguistics.

Dai Quoc Nguyen, Thanh Vu, Tu Dinh Nguyen, Dat Quoc Nguyen, and Dinh Phung. 2019. A Capsule Network-based Embedding Model for Knowledge Graph Completion and Search Personalization. In Proceedings of the 2019 Annual Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies (NAACL-HLT), pages 2180–2189.

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, pages 1955–1961. AAAI Press.
Maximilian Nickel and Volker Tresp. 2013. Tensor factorization for multi-relational learning. In *Machine Learning and Knowledge Discovery in Databases*, pages 617–621, Berlin, Heidelberg. Springer Berlin Heidelberg.

Jeffrey Pennington, Richard Socher, and Christopher Manning. 2014. Glove: Global vectors for word representation. In *Proceedings of the 2014 conference on empirical methods in natural language processing (EMNLP)*, pages 1532–1543.

Michael Schlichtkrull, Thomas N Kipf, Peter Bloem, Rianne van den Berg, Ivan Titov, and Max Welling. 2017. Modeling relational data with graph convolutional networks. *arXiv preprint arXiv:1703.06103*.

Chao Shang, Yun Tang, Jing Huang, Jinbo Bi, Xiaodong He, and Bowen Zhou. 2019. End-to-end structure-aware convolutional networks for knowledge base completion.

Fabian M. Suchanek, Gjergji Kasneci, and Gerhard Weikum. 2007. Yago: A Core of Semantic Knowledge. In *16th International Conference on the World Wide Web*, pages 697–706.

Zhiqing Sun, Zhi-Hong Deng, Jian-Yun Nie, and Jian Tang. 2019. Rotate: Knowledge graph embedding by rotational rotation in complex space. In *International Conference on Learning Representations*.

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 *Proceedings of the 33rd International Conference on International Conference on Machine Learning - Volume 48*, ICML'16, pages 2071–2080. JMLR.org.

Haoyu Wang, Vivek Kulkarni, and William Yang Wang. 2018. DOLORES: deep contextualized knowledge graph embeddings. *CoRR*, abs/1811.00147.

Zhen Wang, Jianwen Zhang, Jianlin Feng, and Zheng Chen. 2014. Knowledge graph embedding by translating on hyperplanes. In *Proceedings of the Twenty-Eighth AAAI Conference on Artificial Intelligence, AAAI’14*, pages 1112–1119. AAAI Press.

Han Xiao, Minlie Huang, and Xiaoyan Zhu. 2016. Transg : A generative model for knowledge graph embedding. In *Proceedings of the 54th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 2316–2325. Association for Computational Linguistics.

Jun Wen Yuan, Neng Gao, and Ji Xiang. 2019. Transgate: Knowledge graph embedding with shared gate structure. In *AAAI*.