On Evaluating Embedding Models for Knowledge Base Completion

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ABSTRACT
Knowledge bases contribute to many web search and mining tasks, yet they are often incomplete. To add missing facts to a given knowledge base, various embedding models have been proposed in the recent literature. Perhaps surprisingly, relatively simple models with limited expressiveness often performed remarkably well under today’s most commonly used evaluation protocols. In this paper, we explore whether recent models work well for knowledge base completion and argue that the current evaluation protocols are more suited for question answering rather than knowledge base completion. We show that when focusing on a different prediction task for evaluating knowledge base completion, the performance of current embedding models is unsatisfactory even on datasets previously thought to be too easy. This is especially true when embedding models are compared against a simple rule-based baseline. This work indicates the need for more research into the embedding models and evaluation protocols for knowledge base completion.

KEYWORDS
Embedding Models, Relational Learning, Evaluation

1 INTRODUCTION
Knowledge bases (KB) such as DBpedia [3] or YAGO [19] have become valuable resources for many web applications, including web search [23, 30], information extraction [13], and question answering [1, 10, 31]. A knowledge base is a collection of relational facts, often represented in form of (subject, relation, object)-triples; e.g., (Einstein, bornIn, Ulm). Despite the great effort in constructing large KBs, they still miss a large number of facts [29]. Consequently, there has been considerable interest in the task of knowledge base completion (KBC), which aims to automatically infer missing facts by reasoning about the information already present in the KB.

In the recent literature, a large number of embedding models for KBC have been proposed. Such models [17] aim at embedding both entities and relations in a low-dimensional latent factor space such that the structure of the knowledge graph is suitably captured. The embeddings are subsequently used to score unobserved triples in order to assess whether they constitute missing information (high score) or are likely to be false (low score). Liu et al. [14] and Wang et al. [28] recently showed that some embedding models are restricted in expressiveness in the sense that they cannot model all types of relations, most notably TransE [4] and DistMult [32]. Nevertheless, these models showed competitive empirical results in multiple studies. Moreover, it was repeatedly shown that simple baselines outperformed the best embedding models for KBC, raising concerns about the benchmarks [25], the models [12] and the evaluation [11].

In this paper, we argue that the methods used to evaluate these models are more suitable for question answering (QA) than for KBC. The most commonly used evaluation protocol [2] for KB embedding models is the entity ranking protocol (ER), which uses held-out test data to assess model performance. In particular, for each true test triple such as (Einstein, bornIn, Ulm), the embedding model is used to rank answers to the questions (?, bornIn, Ulm) and (Einstein, bornIn, ?). Model performance is then assessed based on the rank of the test triple in the result. ER thus assesses a model’s performance for KBC based on its ability to answer certain questions. The evaluation set is constructed such that these questions are “sensical” and they always have an answer. As a result, models that assign high scores to nonsensical triples such as (Ulm, bornIn, Einstein) are not penalized because the corresponding questions are never asked.

Unlike QA, where the focus is on answering meaningful questions, KBC has different goals: (1) to add missing true triples to the knowledge base and (2) to avoid adding false triples. The first point relates to recall, while the second relates to precision. In fact, a model that performs well under ER may have low precision overall, i.e., it may assign high scores to a large number of false triples (e.g., nonsensical triples). If we completed a KB using the high-scoring triples, we would add these false triples and deteriorate precision. This is undesirable, since many KBs are constructed to be highly precise—e.g. YAGO has a precision of 95% [24]—and a drop in precision would negatively affect downstream applications. Thus, models that assign high scores to false triples should be penalized.

In this paper, we propose that instead of asking (i, k, ?) and (?, k, j), a more appropriate question for KBC is (?, k, ?), e.g. (?, bornIn, ?), since in KBC we are interested in any missing facts for every relation k. To estimate the performance of the models when answering such questions, we explore a new protocol for automatic evaluation called entity-pair ranking (PR). For a given relation k, PR

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1 We discuss other less adopted evaluation methods in Sec. 3.2.
ranks answers to the question (?, k, ?), e.g. (?, bornIn, ?), meaning that the rank of all test triples of relation bornIn are compared against all possible answers, i.e., entity pairs in the knowledge graph. This includes nonsensical triples such as (Ulm, bornIn, Einstein). Consequently, model performance when evaluating with PR is negatively affected when models assign high scores to false or even nonsensical triples.

The central research question in this work is: do embedding models work well for KBC? To that end, we conducted an extensive set of experiments to evaluate the performance of well-known embedding models on multiple datasets using ER and PR. When comparing embedding models with a simple rule-based approach on standard datasets, we found that PR generally shows the performance of all models to be unsatisfactory for KBC, which is unlike what is suggested by ER. Additionally, we analyzed the underestimation effect present in all evaluation protocols due to unobserved true triples predicted by the models. This issue is inherent in KBC and it is generally unavoidable for automatic methods, i.e. without human labeling. We found that while PR suffers from this effect as well, it can still be useful to assess model performance for KBC. Finally, we argue that the performance of embedding models was mostly due to the nonsensical triples considered in PR, we applied the background knowledge of domain-range constraints to filter out many of these clearly nonsensical triples. We found that embedding models indeed suffer from nonsensical triples, and that their performance is still unsatisfactory even after removing these triples during evaluation.

Our results indicate that entity ranking is not suitable for KBC, as it considerably overestimates the performance of embedding models. In addition, we observed that when compared against a simple rule-based baseline, current embedding models do not perform well even on “simple” datasets. This implies the need for more powerful models. To the best of our knowledge, this is the first work which elaborates on the problems of current evaluation protocols, and shows that current embedding models have unsatisfactory performance even on the benchmark datasets which were thought to be too easy for embedding models.

This paper is organized as follows: in Section 2 we introduce the basic concepts of embedding-based, as well as rule-based models for KBC. In Section 3 we describe the currently used evaluation protocols for KBC, discuss their shortcomings, and propose an alternative protocol for the experimental study in Section 4. We draw conclusions in Section 5.

2 PRELIMINARIES

Given a set of entities $\mathcal{E}$ and a set of relations $\mathcal{R}$, a knowledge base $\mathcal{K} \subseteq \mathcal{E} \times \mathcal{R} \times \mathcal{E}$ is a set of triples $(i, k, j)$, where $i, j \in \mathcal{E}$ and $k \in \mathcal{R}$. Commonly, $i, k$ and $j$ are referred to as the subject, relation, and object, respectively. A knowledge base can be viewed as a labelled graph, where each vertex corresponds to an entity, each label to a relation, and each labeled edge to a triple.

An embedding model associates an embedding $e_i \in \mathbb{R}^d$ and $r_k \in \mathbb{R}^{d_k}$ in a low-dimensional vector space with each entity $i$ and relation $k$, respectively. We refer to hyperparameters $d, d_k \in \mathbb{N}^+$ as the size of the embeddings. Each model uses a scoring function $s : \mathcal{E} \times \mathcal{R} \times \mathcal{E} \rightarrow \mathbb{R}$ to associate a score $s(i, k, j)$ to each triple $(i, k, j) \in \mathcal{E} \times \mathcal{R} \times \mathcal{E}$. The scores induce a ranking: triples with high scores are considered more likely to be true than triples with low scores. The scoring function depends on $i$, $k$, and $j$ only through their respective embeddings $e_i$, $r_k$, and $e_j$. Roughly speaking, the models try to find embeddings that capture the structure of the entire knowledge graph well. Since embeddings constitute a form of compression, the models are forced to generalize so that new facts can be predicted.

In the following, we briefly review some recent embedding models for knowledge base completion. We focus throughout on the set of models investigated with respect to their expressiveness in Liu et al. [14], Wang et al. [28]. This allows us to compare model expressiveness with empirical model performance. Many more models have been proposed in the literature; e.g. the neural models GCN [20] and ConvE [6].

Embedding models. We subsequently write $R_k \in \mathbb{R}^{d \times d}$ (instead of $r_k$) for the embedding of relation $k$ if it is best interpreted as a matrix. Then $d_R = d^2$; otherwise, $d_R = d$.

RESCAL [18] is the most general bilinear model and uses the scoring function $s(i, k, j) = e_i^T R_k e_j$. TransE [4] is a translation-based model inspired by Word2Vec [16] and uses the score function $s(i, k, j) = -\|e_i + r_k - e_j\|$ (using either $l_1$ or $l_2$ norm). DistMult [5, 32] is a fairly constrained factorization model with scoring function $s(i, k, j) = e_i^T \text{diag}(r_k) e_j$. ComplEx [27] uses embeddings in the complex domain with scoring function $s(i, k, j) = \text{Real}(e_i^T \text{diag}(r_k) e_j)$, where $\text{Real}()$ extracts the real part of a complex number. Algebra [14] uses the scoring function $s(i, k, j) = e_i^T R_k e_j$ of RESCAL, but constrains $R_k \in \mathbb{R}^{d \times d}$ to a block diagonal matrix in which each block is either a real scalar or a $2 \times 2$ matrix of form $\begin{pmatrix} x & -y \\ y & x \end{pmatrix}$ with $x, y \in \mathbb{R}$.

Unlike RESCAL, Algebra and ComplEx, DistMult and TransE are restricted models in that they cannot represent any given knowledge base. See Sec. 3.2 for more details.

Rule learning. A traditional approach to relational tasks is rule learning [9]. Recent examples of successful rule learning systems are AMIE and RuleN [8, 15]. Generally speaking, such an approach learns rules which encode dependencies found in the KB. The types of rules a given system can learn are known as its language bias. Specific rules are learned by looking at groundings of these possible rules in the data. These instances will determine the rule’s confidence. Subsequently, the learned probabilistic rules are used in combination with the KB to predict missing facts based on their assigned scores.

3 EVALUATION PROTOCOLS

Previous work questioned the effectiveness of benchmark datasets [6, 25]. In contrast, in this section we point out the issues with the current evaluation protocols for KBC. To this end, we first review two widely used evaluation protocols. We then argue that these protocols are not well-suited for assessing KBC performance, because they focus on a small subset of all possible facts for a given relation, and thus the overall precision of the models is not reflected in the results. To illustrate this point, we describe the PR protocol and discuss its advantages and potential shortcomings.
3.1 Current Evaluation Protocols

Most studies use the triple classification (TC) and the entity ranking (ER) protocols to assess model performance, where ER is arguably the most widely adopted protocol. We assume throughout that only true but no false triples are available (as is commonly the case), and that these triples are divided into training, validation, and test triples. The union of these three sets acts as a proxy of the entire KB, which is unknown due to incompleteness.

Triple classification (TC). The goal of TC is to test the model’s ability to discriminate between true and false triples [22]. Since only true triples are available in practice, pseudo-negative triples are generated by randomly replacing either the subject or the object of each test triple by another random entity that appears as a subject or object, respectively. Each resulting triple is then classified as positive or negative. In particular, triple \((i, k, j)\) is classified as positive if its score \(s(i, k, j)\) exceeds a relation-specific decision threshold \(\sigma_k\) (learned on validation data using the same procedure). Model performance is assessed by its accuracy, i.e., how many triples are classified correctly.

Entity ranking (ER). The goal of ER is to assess model performance in terms of ranking answers to certain questions. In particular, for each test triple \(t = (i, k, j)\), two questions \(q_k = (?, k, j)\) and \(q_0 = (i, k, ?)\) are generated. For question \(q_k\), all entities \(i' \in \mathcal{E}\) are ranked based on the score \(s(i', k, j)\). To avoid misleading results, entities \(i'\) that correspond to observed triples in the dataset (i.e., \((i', k, j)\) in train/validate) are discarded to obtain a filtered ranking. The same process is applied for question \(q_0\). Model performance is evaluated based on the recorded positions of the test triples in the filtered ranking. The intuition is that models that rank test triples (which are known to be true) higher are expected to be superior. Usually, the micro-average of filtered \(\text{Hits}_@K\)—i.e., the proportion of test triples ranking in the top-\(K\)—and filtered \(\text{MRR}\)—i.e., the mean reciprocal rank of the test triples—are reported. Figure 1a provides a pictorial view of ER for a single relation. Given the score matrix of a relation \(k\), where \(s_{ij}\) is the score of triple \((i, k, j)\), a single test triple is shown in green, all candidate triples considered during the evaluation are shown in blue, and all triples observed in the training, validation and testing sets (not considered during evaluation) are shown in grey.

3.2 Discussion

Regarding triple classification, Wang et al. [28] found that most models achieve an accuracy of at least 93%. This is due to the fact that negative triples with high score are rarely sampled as pseudo-negative triples because of the large number of entities from which the single replacement entity is picked for a given test triple. This means that most classification tasks are “easy”. Consequently, the accuracy of triple classification overestimates model performance for KBC tasks. This protocol is less adopted in recent work.

We argue that ER also overestimates model performance for KBC. In particular, the protocol is more appropriate to evaluate question answering tasks. Since ER generates questions from true test triples, it only asks questions that are known to have an answer. The question itself leaks this information from the test data into the evaluation. This is fine for QA, where the assumption that only “sensical” questions are asked is suitable. In KBC, however, our goal is to infer missing triples with high precision. Consequently, models need to assess every candidate triple, even nonsensical ones such as \((\text{Algorithms to Live By}, \text{visit}, \text{Turing Award})\), because they should be accurate on these as well.

To better illustrate why ER can lead to misleading results, consider the DistMult model and the asymmetric relation \(\text{nominatedFor}\). As described in Sec. 2, DistMult models all relations as symmetric in that \(s(i, k, j) = s(j, k, i)\). Now consider triple \(t = (H. \text{Simon}, \text{nominatedFor}, \text{Nobel Prize})\), and let us suppose that the model successfully assigns \(t\) a high score \(s(t)\). Then the inverse triple \(t' = (\text{Nobel Prize}, \text{nominatedFor}, H. \text{Simon})\) will also obtain a high score since \(s(t') = s(t)\). Thus, if we use DistMult for KBC, either both or none of these triples will be added to the KB: in each case, we make an error. In ER, however, we never ask a question about \(t'\) since there is no test triple for this relation containing either \(\text{Nobel Prize}\) as subject or \(H. \text{Simon}\) as object, so these errors made by DistMult do not affect its overall performance. Thus the symmetry property of DistMult does not influence the result.

For another example, consider TransE and the lexical relation \(k = \text{derivationally related form}\), which is symmetric but not reflexive.

![Figure 1: Triples considered during the evaluation by both protocols. In ER, the evaluation is performed for each test triple separately. In PR, all test triples for a given relation are considered simultaneously. Notice that the unobserved triple \(s_{nj}\) is not a candidate in ER for test triple \(s_{ij}\).](image)
We propose an alternative protocol called Entity-Pair Ranking (PR).

are proportional to the number of test triples

\[ \text{Hits@K} \]

weighted mean average precision in the top-

The number of candidates is much higher than those considered

bounded by \( K \). PR does not rely on MRR for PR, but consider weighted

MAP@K

\[ \left| \mathcal{T}^\text{valid} \right| \]

\[ \left| \mathcal{T}^\text{test} \right| \]

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|c|}
\hline
Dataset & |\( \mathcal{E} \)\] & |\( \mathcal{R} \)\] & |\( \mathcal{T}^\text{train} \)\] & |\( \mathcal{T}^\text{val} \)\] & |\( \mathcal{T}^\text{test} \)\] \\
\hline
FB15K & 14 951 & 1 345 & 483 142 & 50 000 & 59 071 \\
FB-237 & 14 505 & 237 & 272 115 & 17 535 & 20 466 \\
WN18 & 40 943 & 18 & 141 442 & 5 000 & 5 000 \\
WNRR & 40 559 & 11 & 86 835 & 2 824 & 2 924 \\
\hline
\end{tabular}
\caption{Dataset statistics}
\end{table}

Note that all evaluation methods for KBC may underestimate model performance. This happens when models rank unobserved true triples (neither in train/validate/test) high. This behaviour is generally unavoidable for any protocol without further background knowledge or manual labelling, but it may be of particular importance in this protocol due to the large number of candidates considered. We empirically study this underestimation effect in PR in Sec. 4.4.

Another concern about the entity-pair ranking protocol is its computation cost. There are \(|\mathcal{E}|^2\) possible entity pairs to consider per relation, and it may be infeasible to compute the score of all these pairs when there is a large number of entities. Note, however, that the protocol only makes use of the high-scoring entity pairs. Such entity pairs may be determined more efficiently, e.g., using techniques for maximum inner-product search such as Shrivastava and Li [21] or by exploiting available background knowledge as in Sec. 4.5. Moreover, even when the scores of all entity pairs have to be computed, one does not have to sort all the scores to obtain the sorted top-K. For example, one could use Quickselect to obtain the highest scores and then sort only these. Although we did not run into performance issues in our experimental study, more work into efficient retrieval methods is needed to support larger datasets.

Notice that the confidence of an embedding model of a candidate triple is expressed by the score of that triple. If an embedding model cannot determine which triples are high-scoring, it is unclear how to produce candidate triples to add to the KB. Thus, in general, if we cannot determine high-scoring triples from a particular embedding model, then that embedding model may not be suitable for KBC in the first place. Following this argument, a metric based on only top-K candidates suits better than a holistic one based on the ranking of all candidates for KBC, since a model which predicts well for top-K but performs weakly in terms of the whole ranking is still useful for KBC.

### 3.3 Entity-Pair Ranking Protocol

We propose an alternative protocol called Entity-Pair Ranking (PR). While PR may not be the final solution for automatic evaluation, it is still helpful to answer our research question, as we will see in the next section. PR is simple: for each relation \( k \), we ask question \((?, k, ?)\). As before, we use the model to rank all answers, i.e., pairs of entities, and filter out training and validation data in the ranking so as to rank only triples not used during model training. In this way, any negative triples with a high score will appear at a top position, making it harder for true triples to rank high. Figure 1b shows the contrast between the number of negative triples considered for entity-pair and those considered for ER. Again, test triples are shown in green, candidate triples are shown in blue, and triples observed during training and validation are shown in grey.

The number of candidates is much higher than those considered for ER. However, when answering the question \((?, k, ?)\) with all possible entity pairs, all test triples for relation \( k \) will be ranked simultaneously. Let \(|\mathcal{T}_k|\) be the number of test triples in \( k \). ER needs to consider in total \( 2 \cdot |\mathcal{T}_k| \cdot |\mathcal{E}| - 1 \) candidates for \( k \), while PR needs to consider \(|\mathcal{E}|^2\) candidates.

Since all test triples in relation \( k \) are considered at once, we do not rely on MRR for PR, but consider weighted MAP@K, i.e., weighted mean average precision in the top-K filtered results, and weighted Hits@K, i.e., weighted percentage of test triples in the top-K filtered results. For a fixed \( K \), the weights for each relation \( k \) are proportional to the number of test triples |\( \mathcal{T}_k \)| and upper bounded by \( K \):

\[
\text{MAP@K} = \sum_{k \in \mathcal{R}} \text{AP}_k@K \times \frac{\min(|\mathcal{E}|, |\mathcal{T}_k|)}{\sum_{k' \in \mathcal{R}} \min(|\mathcal{E}|, |\mathcal{T}_{k'}|)}
\]

\[
\text{Hits@K} = \sum_{k \in \mathcal{R}} \text{Hits}_k@K \times \frac{\min(|\mathcal{E}|, |\mathcal{T}_k|)}{\sum_{k' \in \mathcal{R}} \min(|\mathcal{E}|, |\mathcal{T}_{k'}|)}
\]

where AP\_K@K is the average precision of the top-K list with respect to the test tuples and Hits\_K@K corresponds to the ratio of test triples in the top K (i.e., (# test triples in top-K)/min(K, |\( \mathcal{T}_k \)|)). In a nutshell, infrequent relations are not treated the same as frequent ones during evaluation due to the weighting factor.

4 EXPERIMENTAL STUDY

We conducted experiments to study the performance of various embedding models for KBC. As baseline, we consider a very simple system called RuleN [15], as it has shown good performance according to the existing entity ranking results. Our goal was not to determine which model currently works best, but rather to determine whether they are suitable for KBC when asking the question \((?, k, ?)\). In addition, we investigated the extent to which the underestimation effect due to unobserved triples affects PR. Finally,
We will see that despite their simplicity, these datasets can still shed light on the behavior of various models under PR. WN18, FB-237, and WNRR. The first two are subsets of WordNet and Freebase, respectively [4], and it is known that the regularities in the datasets can be explained via simple implication rules [6, 15]. We will see that despite their simplicity, these datasets can still shed some light on the behavior of various models under PR. FB-237 is constructed from FB15K to make the dataset more challenging [26], and model performance is indeed considerably lower [2]. Let $\mathcal{T}_{\text{train}}, \mathcal{T}_{\text{val}}, \mathcal{T}_{\text{test}}$ be the training, validation, and test data, resp. Then FB-237 is obtained from FB15K by removing inverse relations and by ensuring that whenever $(i, k, j) \in \mathcal{T}_{\text{test}} \cup \mathcal{T}_{\text{val}}, (i, k', j) \not\in \mathcal{T}_{\text{train}}$ for all $k' \neq k$. WNRR is constructed from WN18 by following similar procedure. Key dataset statistics are summarized in Table 1. Interestingly, the latter two datasets were created when considering the former two datasets unsuitable for the task. Conversely, we suggest that independent of the dataset, the standard evaluation protocol in unsuitable.

Negative sampling. Since we are only given true but no false triples, embedding models are usually trained using a negative sampling strategy to obtain pseudo-negative triples [17]. We consider three sampling strategies in our experiments: 

- **Perturb 1**: For each training triple $t = (i, k, j)$, sample each pseudo-negative triple by randomly replacing either $i$ or $j$ by a random entity (such that the resulting triple is unobserved). This ensures that at least one entity is observed in the training data of relation $k$, which to some extent avoids nonsensical pseudo-negative triples.

- **Perturb 2**: For each training triple $t = (i, k, j)$, sample each pseudo-negative triple by sampling random unobserved tuples from relation $k$. This method produces many nonsensical negative triples, but is more suited to KBC, which is based on the question $(?, k, ?)$. 

- **Perturb 1-R**: For each training triple $t = (i, k, j)$, sample each pseudo-negative triple by randomly replacing either $i$, $k$ or $j$ by a random entity (or relation for $k$). The generated negative samples are not compared with the training set [14].

Training and implementation. We trained all embedding models as in previous work [4, 27]. In particular, we used AdaGrad [7] as an optimizer and trained DistMult, ComplEx, Analogy and RESCAL with binary cross-entropy loss, which works well in practice. TransE always produces negative scores, so it is unclear how to train it with cross-entropy loss in a principled way. We thus used pair-wise ranking loss with margin $\gamma \geq 0$ as in Bordes et al. [4]. We implemented all embedding models on top of the code from Liu et al. [14] in C++ using OpenMP. For RuleN, we use the original implementation provided by the authors. The evaluation protocols were written in Python, with Bottleneck\(^3\) used for efficiently obtaining the top K entries in a given score matrix, such that only these entries required sorting.

Hyperparameters. The best hyperparameters are selected based on MRR (for ER) and MAP@100 (for PR) on the validation data. These are reported for both evaluation protocols in the appendix. For both protocols, we performed an exhaustive grid search over the following hyperparameter settings: $d \in \{100, 150, 200\}$, weight of $l_2$-regularization $\lambda \in \{0.1, 0.01, 0.001\}$, learning rate $\eta \in \{0.01, 0.1\}$, negative sampling strategies Perturb 1, Perturb 2 and Perturb 1-R, and margin hyperparameter $\gamma \in \{0.5, 1, 2, 3, 4\}$ for TransE. For each training triple, we sampled 6 pseudo-negative triples. To keep effort tractable, we only used the most frequent relations from each dataset for hyperparameter tuning (top-5, top-5, top-15, and top-30 most frequent relations for WN18, WNRR, FB-237 and FB-15k respectively).\(^4\) We trained each model for up to 500 epochs during grid search (1800 for TransE).\(^5\) In all cases, we used early stopping, i.e., we evaluated model performance every 50 epochs and used the overall best-performing model. The best hyperparameters for both evaluation protocols are reported in the online material. We found that Perturb-2 can indeed be useful in both protocols. RuleN learns path rules of a given length and a particular type of constant rules. Moreover, RuleN takes a sample of the KB when looking for groundings of rules. We refer to Meilicke et al. [15] for the details. We use the best settings reported by the authors with respect to entity ranking [15]. That is, for FB15K and FB-237, we learned path rules of length 2 and constant rules, and the sampling size was set to 1000. For WN18 and WNRR, we learned path rules of length 2 with sampling size of 1000, and path rules of length 3 with sampling size of 100, as well as constant rules. For PR, we learned path rules of length 2 using a sampling size of 500 for FB15K and FB-237. For WN18 and WNRR, we learned path rules of length 3 and set the sampling size to 500.

### 4.2 Performance Results with ER

Table 2 summarizes our results with ER. Embedding models perform competitively with respect to RuleN on all datasets, except for their MRR performance on FB15K. Notice that this generally holds even for the more restricted models (TransE and DistMult) on the more challenging datasets, which were created after criticizing FB15K and WN18 as too easy [6, 25]. Due to such results, DistMult is considered a state-of-the-art model for KBC [12]. This seems counterintuitive (especially considering the more difficult datasets), since DistMult can only model symmetric relations, but most relations in these datasets are asymmetric. Regarding TransE, while its MRR was relatively low on all datasets except FB-237, it still achieved great performance in Hits@10. Again, this is counterintuitive because WN18 contains a large number of symmetric relations, so it should be difficult for TransE to achieve good results. These observations indicate that ER may not be well-suited for KBC.

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\(^3\)https://github.com/quark0/ANALOGY

\(^4\)All datasets are highly skewed.

\(^5\)Chosen such that models are usually converged.
4.3 Performance Results with PR

The evaluation results of PR with \( K = 100 \) are summarized in Table 3. Note that Tables 2 and 3 are not directly comparable, because PR considers all test triples for a given relation simultaneously. Consequently, it is more difficult to rank at the top in PR, so we chose \( K > 10 \). Performance for different values of \( K \) is reported in Fig. 2. Also, recall that for ER we compute MRR, while for PR we compute MAP, as explained in Sec. 3.3. The effect of the choice of \( K \) is discussed later in this section.

For now, assume that there is no unobserved true triples other than the test set. We defer the discussion of this issue in Sec. 4.4. Since knowledge bases strive for high accuracy, we consider models unsatisfactory if we cannot use them to add new facts without sacrificing this accuracy throughout this section. For the embeddings, observe that the performance of all models is unsatisfactory on all datasets, especially when compared with RuleN on FB15K and WN18, which were previously considered to be too easy for embedding models. Specifically, DistMult’s Hits@100 is slightly less than 10% on WN18, meaning that if we add the top 100 ranked triples to the KB, over 90% of what is added is likely false. Even when using ComplEx, the best model on FB15K, we would potentially add more than 50% false triples. This implies that embedding models cannot even capture simple rules successfully. The notable exceptions are Analogy and ComplEx on WN18. TransE and DistMult did not achieve competitive results on WN18, even when compared with other embedding models. In addition, DistMult did not achieve competitive results on FB15K and FB-237 and TransE did not achieve competitive results in WNRR. When considering all datasets, there was no single embedding model which outperformed all others. In general, ComplEx and Analogy achieved consistently better results across different datasets than other models. But when compared with the baseline, even the performance of these models was often not satisfactory. This suggests that better models and/or training strategies are needed for embedding models.

With respect to FB-237 and WNRR, it is intrinsically difficult for rule-based approaches to learn simple rules with high confidence because of the way these datasets were constructed [15]. As a result, RuleN does not perform well on these two datasets. This is reflected both by ER and PR.

To better understand the behavior of TransE and DistMult, we investigated their performance on the top-5 most frequent relations on WN18. Table 4 shows the number of test triples appearing in the top-100 list. We found that the norm of the embedding vector of this relation was 0.1, which was considerably smaller than for the other relations (avg. 1.4). This supports our argument that TransE has a tendency to push symmetric relations embeddings to 0.

Note that while hypernymy, hyponymy, member meronym, and member holonym are semantically transitive, the dataset contains almost exclusively their transitive core, i.e., the dataset (both train and test) does not contain many of the transitive links of the relations. As a result, the models do not “see” their transitivity. Thus, models that cannot handle transitivity well may still produce good results. This might explain why TransE performs better for these relations than for derivationally related form. DistMult did not perform well on these relations (they are asymmetric). ComplEx and Analogy showed superior performance across all relations. RESCAL

| Dataset | FB15K MRR (%) Hits@K (%) | FB-237 MRR (%) Hits@K (%) | WN18 MRR (%) Hits@K (%) | WNRR MRR (%) Hits@K (%) |
|---------|--------------------------|---------------------------|------------------------|------------------------|
| DistMult | 66.0 84.5                | 27.0 43.2                 | 79.0 93.7              | 43.2 47.4              |
| TransE  | 50.0 77.7                | 29.0 46.6                 | 72.0 90.8              | 22.0 49.1              |
| ComplEx | 67.2 83.3                | 28.0 43.5                 | 94.0 94.8              | 44.0 48.1              |
| Analogy | 67.0 83.8                | 27.0 43.3                 | 94.1 94.2              | 44.0 48.6              |
| RESCAL  | 44.4 68.7                | 27.0 42.7                 | 92.0 93.9              | 42.0 44.7              |
| RuleN   | 80.5 87.0                | 26.0 42.0                 | 95.0 95.8              | — 53.6                 |

Table 2: Results with the commonly used entity ranking protocol (ER) \( (K = 10) \)

| Dataset | FB15K MAP@K (%) Hits@K (%) | FB-237 MAP@K (%) Hits@K (%) | WN18 MAP@K (%) Hits@K (%) | WNRR MAP@K (%) Hits@K (%) |
|---------|--------------------------|---------------------------|------------------------|------------------------|
| DistMult | 1.3 10.4                 | 0.3 4.2                   | 7.9 9.7                | 14.1 17.8              |
| TransE  | 21.1 36.3                | 7.9 17.6                  | 22.3 31.5              | 0.2 1.3                |
| ComplEx | 25.9 45.2                | 7.1 16.6                  | 78.5 87.7              | 16.8 20.0              |
| Analogy | 18.8 34.8                | 4.9 14.3                  | 61.5 75.8              | 15.4 19.8              |
| RESCAL  | 15.0 30.3                | 6.7 15.0                  | 48.2 60.9              | 13.1 13.8              |
| RuleN   | 77.4 83.7                | 7.6 15.8                  | 94.8 96.8              | 21.5 25.1              |

Table 3: Results with the proposed entity-pair ranking protocol (PR) \( (K = 100) \)
is in between, most likely due to difficulties in finding a good parameterization. However, it is unclear why TransE performs well on FB15K and FB-237.

To investigate the performance of models for different values of $K$, we give the curves of Hits@$K$ and MAP@$K$ as a function of $K$ for all datasets in Fig. 2 and Fig. 3 respectively. ComplEx and Analogy performed best for large $K$ w.r.t. other embedding models. Similarly, TransE works the best for small values of $K$ on FB15K and FB-237. Notice that RuleN performs considerably better on FB15K, WN18 and WNRR, while it still performs competitively on FB-237.

Regarding runtimes, we found that PR is 3 to 4 times slower than ER, but still manageable for these datasets (30–90 minutes in general).

### 4.4 Influence of Unobserved True Triples

Since all datasets are based on incomplete knowledge bases, evaluation protocols may systematically underestimate model performance. For ranking-based evaluations in particular, a true triple that is neither in the training, nor validation, nor test data may be ranked high by some model, but we treat that triple as negative during the evaluation. Such models would be penalized. In fact, all prior evaluation protocols also have this issue, but PR might be particularly sensitive to this due to the large number of candidates considered during evaluation.

Generally, it is unclear how to design an automatic evaluation strategy that avoids this problem. Manual labeling can be used to address this, but it may sometimes be infeasible given the large number of relations, entities, and models for KBC. Moreover, depending on the domain of the data, such labeling may even require expert knowledge.

To explore such underestimation effect in PR, we decoded the unobserved triples in the top-100 predictions of the 5 most frequent relations of WN18. We then checked whether those triples are implied by the symmetry and transitivity properties of each relation. In Table 4, we give the resulting number of triples in parentheses (i.e., number of test triples + implied triples). We observed that underestimation indeed happened. TransE was mostly affected, but still did not lead to competitive results when compared to ComplEx and Analogy. RuleN achieves the best possible results in all 5 relations. These results suggest that (1) underestimation is indeed a concern, and (2) the results reported by the PR can nevertheless give an indication of relative model performance.

#### 4.5 Type Filtering

When background knowledge (BK) is available, embedding models only need to predict triples consistent with this BK. Notice that this is inherently what rule-based approaches do, since all predicted candidates will be type-consistent. We explored whether their performance can be improved by filtering out nonsensical triples from each model’s predictions. This should also help reduce computational costs. In particular, we investigated how model performance is affected when we filter out predictions that violate type constraints (domain and range of each relation). If a model performance improves with such type filtering, it must have ranked tuples with incorrect types high in the first place. We can thus assess to what extent models capture entity types as well as the domain and range of the relations.

We extracted from Freebase type definitions for entities and domain and range constraints for relations. We also added the domain (or range) of a relation $k$ to the type set of each subject (or object) entity which appeared in $k$. We obtained types for all entities in both FB datasets, and domain/range specifications for roughly 93% of relations in FB15K and 97% of relations in FB-237. The remaining relations were evaluated as before.

We report in Table 5 the Hits@100 and MAP@100 as well as their absolute improvement (in parentheses) w.r.t. Table 3. We include the results of RuleN from Table 3, since rule-based systems will never predict type-inconsistent facts. The results show that all models improve by type filtering; thus all models do predict triples with incorrect types. In particular, DistMult shows considerable improvement on both datasets. Indeed, about 90% of the relations in

| Relation                     | Model  |
|------------------------------|--------|
| hyponymy                     | DistMult | TransE | ComplEx | Analogy | RESCAL | RuleN |
|                              | 1 (1)   | 18 (32) | 99 (99) | 99 (99) | 92 (93) | 100 (100) |
| hypernymy                    | 0 (0)   | 5 (33)  | 99 (99) | 99 (99) | 96 (98) | 100 (100) |
| derivationally related form  | 100 (100) | 0 (0)  | 100 (100) | 100 (100) | 6 (68)  | 100 (100) |
| member meronym               | 0 (0)   | 18 (41) | 74 (84) | 83 (85) | 44 (63) | 100 (100) |
| member holonym               | 0 (0)   | 16 (47) | 74 (83) | 83 (85) | 37 (54) | 100 (100) |

Table 4: Number of test triples in the top-100 filtered predictions on WN18. An estimate of the number of true triples in the top-100 list is given in parentheses.

| Data   | Model   | MAP@K (%) | Hits@K (%) |
|--------|---------|-----------|------------|
| FB15K  | DistMult| 18.8 (+17.5) | 36.4 (+26.0) |
|        | TransE  | 25.7 (+4.5)  | 41.7 (+5.4)  |
|        | ComplEx | 41.8 (+15.9) | 61.9 (+16.7) |
|        | Analogy | 41.3 (+22.5) | 61.5 (+26.7) |
|        | RESCAL  | 16.7 (+1.7)  | 32.8 (+2.5)  |
|        | RuleN   | 77.4 (0.0)   | 83.7 (0.0)   |
| FB-237 | DistMult| 9.5 (+9.2)   | 18.1 (+13.9) |
|        | TransE  | 11.3 (+3.4)  | 21.2 (+3.6)  |
|        | ComplEx | 11.3 (+4.2)  | 21.8 (+5.2)  |
|        | Analogy | 10.5 (+5.6)  | 20.9 (+6.6)  |
|        | RESCAL  | 10.2 (+3.5)  | 19.0 (+4.0)  |
|        | RuleN   | 7.6 (0.0)    | 15.8 (0.0)   |

Table 5: Results with PR using type filtering (K = 100).
Figure 2: Hits@K with PR as a function of K

Figure 3: MAP@K with PR as a function of K
FB15K (about 85% for FB-237) have a different type for their domain and range. As DistMult treats all relations as symmetric, it introduces a wrong triple for each true triple into the top-\(K\) list on these relations; type filtering allows us to ignore these wrong tuples. This is also consistent with DistMult’s improved performance under ER, where type constraints are implicitly used since only questions with correct types are considered. We also observed that ComplEx and Analogy improved considerably on FB15K. Although it is unclear why this is the case, it implies that the best performing models on this dataset according to ER, are still making a considerable number of type-inconsistent predictions. On FB15K, the relative ranking of the models with type filtering is roughly equal to the one without type filtering. On the harder FB-237 dataset, all models now perform similarly. Notice that when compared with the performance of RuleN, embedding models are still far behind on FB15K, but are no longer behind on FB-237.

Finally, due to the reduction in the number of candidates, the average evaluation time was reduced to about 30% of the time required without BK.

5 CONCLUSION

We investigated the question of whether current embedding models provide good results for the knowledge base completion task. We found that the entity ranking evaluation protocol that is currently widely used is tailored to question answering, but may give a misleading picture of each model’s performance with respect to knowledge base completion, where the aim is high precision. We tested a new and simple evaluation protocol with KBC in mind and evaluated a number of state-of-the-art models under this protocol. We found that most models did not produce satisfactory results, especially when compared against a simple rule-based system used as baseline. This suggests that more research into embedding models and training methods is needed to assess whether, when, and how KB embedding models can provide high-quality results.
APPENDIX

5.1 Hyperparameters of best models

| Data | Model | d   | \(\eta\) | \(\lambda\) | \(\gamma\) | Perturb |
|------|-------|-----|---------|---------|---------|--------|
| FB15K DistMult | 200 | 0.1 | 0.01 | - | 1-R |
| TransE \(_l\) | 100 | 0.1 | - | 2.0 | 1 |
| ComplEx | 200 | 0.1 | 0.001 | - | 1-R |
| Analogy | 200 | 0.1 | 0.001 | - | 1-R |
| RESCAL | 200 | 0.1 | 0.1 | - | 1 |
| FB-237 DistMult | 200 | 0.1 | 0.01 | - | 2 |
| TransE \(_l\) | 100 | 0.1 | - | 4.0 | 1 |
| ComplEx | 200 | 0.1 | 0.01 | - | 2 |
| Analogy | 200 | 0.1 | 0.01 | - | 2 |
| RESCAL | 150 | 0.1 | 0.001 | - | 2 |
| WN18 DistMult | 100 | 0.1 | 0.001 | - | 1 |
| TransE \(_l\) | 150 | 0.1 | - | 4.0 | 1-R |
| ComplEx | 150 | 0.1 | 0.1 | - | 1 |
| Analogy | 200 | 0.1 | 0.001 | - | 1-R |
| RESCAL | 100 | 0.1 | 0.01 | - | 1 |
| WNRR DistMult | 200 | 0.01 | 0.001 | - | 1 |
| TransE \(_l\) | 200 | 0.01 | - | 2.0 | 2 |
| ComplEx | 200 | 0.01 | 0.01 | - | 1 |
| Analogy | 200 | 0.01 | 0.01 | - | 1 |
| RESCAL | 150 | 0.1 | 0.1 | - | 1 |

Table 6: Hyperparameters for best models in ER

| Data | Model | d   | \(\eta\) | \(\lambda\) | \(\gamma\) | Perturb |
|------|-------|-----|---------|---------|---------|--------|
| FB15K DistMult | 200 | 0.1 | 0.001 | - | 2 |
| TransE \(_l\) | 150 | 0.1 | - | 3.0 | 1 |
| ComplEx | 200 | 0.1 | 0.01 | - | 1-R |
| Analogy | 200 | 0.1 | 0.01 | - | 1-R |
| RESCAL | 200 | 0.1 | 0.01 | - | 1-R |
| FB-237 DistMult | 200 | 0.01 | 0.01 | - | 2 |
| TransE \(_l\) | 200 | 0.1 | - | 4.0 | 1 |
| ComplEx | 150 | 0.1 | 0.001 | - | 2 |
| Analogy | 200 | 0.1 | 0.01 | - | 2 |
| RESCAL | 200 | 0.1 | 0.1 | - | 1 |
| WN18 DistMult | 200 | 0.1 | 0.01 | - | 1 |
| TransE \(_l\) | 150 | 0.1 | - | 2.0 | 1-R |
| ComplEx | 200 | 0.1 | 0.01 | - | 1-R |
| Analogy | 150 | 0.1 | 0.01 | - | 1-R |
| RESCAL | 150 | 0.1 | 0.01 | - | 1 |
| WNRR DistMult | 100 | 0.1 | 0.001 | - | 1 |
| TransE \(_l\) | 100 | 0.1 | - | 4.0 | 1-R |
| ComplEx | 200 | 0.1 | 0.001 | - | 1 |
| Analogy | 200 | 0.1 | 0.001 | - | 1 |
| RESCAL | 150 | 0.1 | 0.001 | - | 1-R |

Table 7: Hyperparameters for best models in PR