PromptKG: A Prompt Learning Framework for Knowledge Graph Representation Learning and Application

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ABSTRACT

Knowledge Graphs (KGs) often have two characteristics: heterogeneous graph structure and text-rich entity/relation information. KG representation models should consider graph structures and text semantics, but no comprehensive open-sourced framework is mainly designed for KG regarding informative text description. In this paper, we present PromptKG, a prompt learning framework for KG representation learning and application that equips the cutting-edge text-based methods, integrates a new prompt learning model and supports various tasks (e.g., knowledge graph completion, question answering, recommendation, and knowledge probing). PromptKG is publicly open-sourced at https://github.com/zjunlp/PromptKG with long-term technical support.

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1 INTRODUCTION

Knowledge Graphs (KGs) encode real-world facts as structured data and have drawn significant attention from academia, and the industry [19]. KG representation learning aims to project the relations and entities into a continuous vector space, which can promote the knowledge reasoning ability and feasibly be applied to downstream tasks: question answering [9], recommender system [17] and so on. Previous embedding-based knowledge graph representation methods, such as TransE [2], embed the relational knowledge into a vector space and then optimize the target object by leveraging a pre-defined scoring function to those vectors. A few remarkable open-sourced and long-term maintained KG representation toolkits have been developed, such as OpenKE [5], LibKGE [3], PyKEEN [1], CogKGE [6]. Nevertheless, these embedding-based methods are restricted in expressiveness regarding the shallow network architectures without using any side information.

By comparison, text-based methods [15] incorporate available texts for knowledge representation learning. With the development of prompt learning, lots of text-based models [9, 14] have been proposed, which can obtain promising performance with pre-trained language models (PLMs) and take advantage of allocating a fixed memory footprint for those large-scale real-world KGs. However, there is no comprehensive open-sourced framework particularly designed for KG representation with prompt learning at present,
which makes it challenging to try out new methods and make rigorous comparisons for previous approaches.

In this paper, we share with the community an open-sourced prompt learning framework for KG representation learning and application called PromptKG (MIT License), which supports various cutting-edge text-based KG representation models. Besides, we equip PromptKG with a simple-yet-effective prompt learning method for KG representation learning, which shares the same architecture as normal discrimination PLMs. Empirically, we demonstrate that PromptKG can yield better or comparable performance on seven datasets. We also provide tutorial notebooks for beginners. We will provide maintenance to meet new tasks, new requests, and fix bugs.

2 TEXT-BASED KG REPRESENTATION

In this section, we detail two major types of text-based KG representation (discrimination-based and generation-based) and the proposed prompt learning method for KG representation learning, which are all integrated into PromptKG.

Table 1: Inference efficiency comparison. \(|L|\) is the length of the triple description. \(|L/2|\) can be seen as the length of entity tokens. \(|E|\) and \(|R|\) are the numbers of all unique entities and relations in the graph respectively. Usually, \(|E|\) exceeds hundreds of thousands and is much greater than \(|R|\).

| Model       | PLM    | Support Task | Complexity                  |
|-------------|--------|--------------|-----------------------------|
| KGBERT [15] | MLM    | KGC          | O(|L|²|E|(|R|)                  |
| SimKGC [13] | MLM    | KGC          | O(|L|²|E|(|R+1|)             |
| STAR [12]   | MLM    | KGC          | O(|L|²|E|(|R+1|)             |
| KGT5 [9]    | Seq2Seq| KGC QA       | O(|L|²|E|(|R|)              |
| GenKGC [14] | Seq2Seq| KGC          | O(|L|²|E|(|R|)              |
| kNN-KGE [18] | MLM    | KGC LAMA     | O(|L|²|E|(|R|)              |

**Notation.** Given a triple \((h, r, t)\), we define their natural language descriptions as 
\[X^h = \{x^h_1, x^h_2, ..., x^h_{||h||}\}, X^r = \{x^r_1, x^r_2, ..., x^r_{||r||}\}, X^t = \{x^t_1, x^t_2, ..., x^t_{||t||}\}\]. We denote the embedding of token \(x\) as \(e\).

**Discrimination-based methods.** There are two kinds of models based on the discrimination method: one (e.g., KG-BERT [15], PKGC [7]) utilizes a single encoder to encode triples of KG with text description; others [12, 13] leverage siamese encoder (two-tower models) with PLMs to encode entities and relations respectively. For the first kind, the score of each triple is expressed as:

\[
\text{Score}(h, r, t) = \text{TransformerEnc}(X^h, X^r, X^t),
\]

where TransformerEnc is the BERT model followed by a binary classifier. However, these models have to iterate all the entities to decode sequential schemas and to obtain the embeddings. Then, they use a score function to predict the correct tail entity from the candidates, denoted by:

\[
\text{Score}(h, r, t) = \cos(e(h), e(t)).
\]

**Generation-based methods.** Generation-based models formulate KG completion or other KG-intensive tasks as sequence-to-sequence generation. Given a triple with the tail entity missing \((h, r, ?)\), models are fed with \((X^h, X^r)\) and then output \(X^t\). In the training procedure, generative models maximize the conditional probability:

\[
\text{Score}(h, r, t) = \prod_{i=1}^{|t|} p(x^t_i | x^t_1, x^t_2, ..., x^t_{i-1}; (X^h, X^r))
\]

To guarantee the consistency of decoding sequential schemas and tokens in KG, GenKGC [14] proposes an entity-aware hierarchical decoder to constrain \(X^t\). In addition, inspired by prompt-learning, GenKGC takes triples with the same relation as demonstrations to implicitly encode structured knowledge. Besides, KGT5 [9] proposes to pre-train generation-based PLMs from scratch with text descriptions for KG representation.

A prompt learning method for KG representation learning. We introduce the technical details of the proposed prompt learning method for KG representation learning, which shares the same architecture as normal discrimination PLMs. Note that there are two modules in the normal PLMs: a word embedding layer to embed
We introduce the design principle of PromptKG where

As shown in Figure 1, a unified KG encoder represents graph structure and text semantics; Model Hub: PromptKG is integrated with many cutting-edge text-based KG representation models; Flexible Downstream Tasks: PromptKG disentangles KG representation learning and downstream tasks.

3.1 Unified KG Encoder

As shown in Figure 1, a unified KG encoder represents graph structure and text semantics, supporting different types of text-based KG representation methods. For the discrimination-based method, the input is built on the plain text description as:

\[ X_{\text{head pair}} = [\text{CLS}] X^h [\text{SEP}] X^t [\text{SEP}] \]

\[ X_{\text{tail}} = [\text{CLS}] X^t [\text{SEP}] \]

For the generation-based model, we leverage the tokens in \( X^h \) and \( X^t \) to optimize the model with label \( X^t \). When predicting the head entity, we add a special token \([\text{reverse}]\) in the input sequence for reverse reasoning. Referring to the proposed prompt learning method, we represent entities and relations in KG with special tokens and obtain the input as:

\[ X = [\text{CLS}] X^h [\text{Entity h}] [\text{SEP}] X^t [\text{SEP}] [\text{MASK}] [\text{SEP}] \]

where \([\text{Entity h}]\) represents the special token to the head entity. To encode the graph structure, we sample 1-hop neighbor entities and concatenate their tokens as input for implicit structure information. With such a unified KG encoder, PromptKG can encode both heterogeneous graph structure and text-rich semantic information.

3.2 Model Hub

As shown in Figure 1, PromptKG consists of a Model Hub which supports many representative text-based KG representation models. For example, KG-BERT [15] uses BERT to score the triple with their descriptions. Comparing to its high time complexity, StAR [12] and SimKGC [13] both introduce a tower-based method to pre-compute entity embeddings and retrieve top-\(k\) entities efficiently. Further, GenKGC [14] and KGTS [9] treat knowledge graph completion as sequence-to-sequence generation. Besides, kNN-KGE [18] is a KG representation model which linearly interpolates its entity distribution by \(k\)-nearest neighbors. Note that all the model implementations in Model Hub are modularized; thus, flexible to debug and add new models.

3.3 Applying to Downstream Tasks

We take the proposed prompt learning for KG representation learning as an example and introduce the technical details of applying to downstream tasks as shown in Figure 2. For knowledge graph completion, we feed the model with the textual information \(X^h, X^t\) of the head entity and the relation, then obtain the target tail entity via mask token prediction. For question answering, we feed the model with the question written in natural language concatenated with a \([\text{MASK}]\) token to obtain the special token of the target answer (entity). For recommendation, we take the user’s interaction history as sequential input [10] with entity embeddings and then leverage the mask token prediction to obtain recommended items. For the knowledge probing task, we adopt entity embedding as additional knowledge to help the model better reason through the sentence and predict the token in the masked position following PELT [16].

### Table 2: Hits1 and MRR (%) results on KGC, question answering, recommendation and knowledge probing tasks.

| Task                      | Dataset | Method         | Hits1 | MRR  |
|---------------------------|---------|----------------|-------|------|
| KG Completion             | WN18RR  | KG-BERT        | 4.1   | 21.6 |
|                           |         | StAR           | 24.3  | 40.1 |
|                           |         | SimKGC         | 42.5  | 60.8 |
|                           |         | KGT5           | 17.9  | -    |
|                           |         | GenKGC         | 39.6  | -    |
|                           |         | kNN-KGE        | 52.5  | 57.9 |
|                           | FR15k-237| KG-BERT       | -     | -    |
|                           |         | StAR           | 20.5  | 29.6 |
|                           |         | SimKGC         | 22.6  | 30.1 |
|                           |         | KGT5           | 10.8  | -    |
|                           |         | GenKGC         | 19.2  | -    |
|                           |         | kNN-KGE        | 28.0  | 37.3 |
| Question Answering        | MetaQA  | GT query       | 63.3  | -    |
|                           |         | PubNet         | 65.1  | -    |
|                           |         | KGT5           | 67.8  | -    |
| Recommendation            | ML-20m  | BERTRe          | 34.4  | 47.9 |
|                           |         | PromptKG       | 37.3  | 50.5 |
|                           | TReX    | BERT           | 28.6  | 37.7 |
|                           |         | RoBERTa        | 19.9  | 27.8 |
|                           |         | PromptKG (RoBERTa) | 22.1 | 29.8 |
| Knowledge Probing         | Squad   | BERT           | 13.2  | 23.5 |
|                           |         | RoBERTa        | 13.4  | 24.6 |
|                           |         | PromptKG (RoBERTa) | -   | -    |
|                           | Google RE| BERT           | 10.3  | 17.3 |
|                           |         | RoBERTa        | 7.6   | 12.8 |
|                           |         | PromptKG (RoBERTa) | 8.1 | 14.2 |
|                           | Concept Net| BERT         | 15.1  | 23.1 |
|                           |         | RoBERTa        | 17.8  | 25.4 |
|                           |         | PromptKG (RoBERTa) | -   | -    |

\(^1\)Some models still under fast development in Model Hub can not be directly applied to downstream tasks.
information is a direct downstream task of KG representation; 2) question answering is an intuitive knowledge-intensive task; 3) recommendation involves items aligned to entities in real-world KGs and thus can benefit from KG representation; 4) knowledge probing (LAMA) analyzes the factual and commonsense knowledge contained in language models using cloze-style questions. All datasets and detailed hyper-parameters are all available on the Github for reproducibility.

4.1 Knowledge Graph Completion

For the KG completion task, we conduct link prediction experiments on two datasets WN18RR [4] and FB15k-237 [11], and evaluate the models in PromptKG with hits1 and MRR metrics. From Table 2, we observe that discrimination-based method SimKGC (previous state-of-the-art) achieves higher performance than other baselines. Generation-based models like KG75 [9] and GenKG [14] also yield comparable results and show potential abilities in KG representation. kNN-KGE [18] can obtain promising performance (the best hits1 score) by computing the nearest neighbors based on the distance in the entity embedding space from the knowledge store and a two-step training strategy.

4.2 Question Answering

KG is known to be helpful for the task of question answering. We apply PromptKG to question answering and conduct experiments on the MetaQA dataset. Due to computational resource limits, we only evaluate the 1-hop inference performance. From Table 2, KG75 in PromptKG yields the best performance.

4.3 Recommendation

For the recommendation task, we conduct experiments on a well-established version ML-20m². Linkage of ML-20m and Freebase offered by KB4Rec [20] is utilized to obtain textual descriptions of movies in ML-20m. With movie embeddings pre-trained on these descriptions, we conduct experiments on sequential recommendation task following the settings of BERT4Rec [10]. We notice that PromptKG is confirmed to be effective for the recommendation compared with BERT4Rec.

4.4 Knowledge Probing

Knowledge probing [8] examines the ability of LMs (BERT, RoBERTa, etc.) to recall facts from their parameters. We conduct experiments on LAMA using pre-trained BERT (bert-base-uncased) and RoBERTa (roberta-base) models. To prove that entity embedding enhanced by KGs helps LMs grab more factual knowledge from PLMs, we train a pluggable entity embedding module following PELT [16]. As shown in Table 2, the performance boosts while we use the entity embedding module. Since there is no subject entity annotated in Squad and no URI of the subject entity in ConceptNet for entity alignment, we only apply the entity embedding module to the remaining data in LAMA. PromptKG will support a unified API accessible for enhanced entity embedding in the future.

5 CONCLUSION AND FUTURE WORK

We propose PromptKG, a prompt learning framework for knowledge graph representation learning and application. PromptKG establishes a unified toolkit with well-defined modules and easy-to-use interfaces to support research on using PLMs on KGs. Both for researchers and developers, PromptKG provides effective and efficient training code and supports downstream tasks. In the future, we will continue to integrate more models and tasks (e.g., dialogue) into PromptKG to facilitate the research progress of the KG.

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