Better Learning from Graph Structures: Research on Representation Learning for Knowledge Graph Reasoning

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ABSTRACT

Knowledge graphs (KGs), which store human knowledge facts in intuitive graph structures, are widely used for multiple applications, such as recommendation systems, information retrieval, question and answer, etc. However, as the construction of KGs is always dynamic, the incomplete problem commonly exists no matter which types of KGs they are, further hindering their effectiveness in knowledge representation. To alleviate the problem, knowledge graph reasoning (KGR) has drawn increasing attention these years, aiming to infer missing facts in a given KG. Although existing representation learning models achieve promising performances, the structural information, as the important characteristic between KGs and traditional knowledge bases, should be better leveraged. To this end, my PhD research targets representation learning for KGR by designing effective mechanisms to better utilize the information underlying the graph structures in KGs and achieve several progresses. Beyond my current research scope, I find that there are two key problems restricting the development of KGR, *i.e.,* efficiency, and the way to cooperate with LLMs, which I plan to work on in the future.

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1 INTRODUCTION

Knowledge graphs (KGs), which store the human knowledge facts in intuitive graph structures [5], are widely used for multiple applications, such as information retrieval [12, 18], question and answering [21], etc. Current KGs can be roughly divided into three types, *i.e.,* static KGs, temporal KGs and multi-modal KGs, as shown in Fig. 1. Although the basic KGs, storing the knowledge only as static uni-modal facts, are powerful and expressive, they cannot fully describe real-world scenarios, which contain information from various sources [9]. Thus, two more practical KGs have been proposed recently, *i.e.,* temporal KGs and multi-modal KGs, where temporal and multi-modal information are integrated with basic KGs. However, as the construction of KGs is always dynamic [9], the incomplete problem commonly exists no matter which types of KGs they are, further hindering their effectiveness in knowledge representation. To alleviate the problem, knowledge graph reasoning (KGR) has drawn increasing attention these years, aiming to infer missing facts in a given KG.

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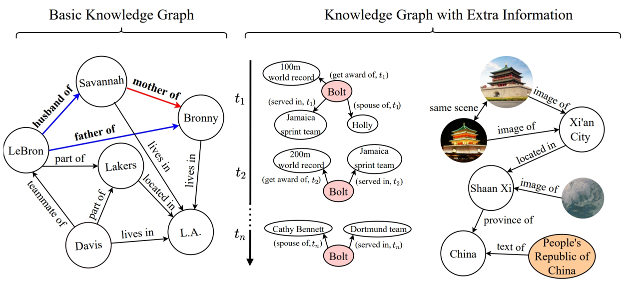

(a) Static Knowledge Graph (b) Temporal Knowledge Graph (c) Multi-Modal Knowledge Graph

Figure 1: Examples of three categories of the knowledge graphs, *i.e.,* static knowledge graphs, temporal knowledge graphs, and multi-modal knowledge graphs [9].

The KGR models can be categorized into two types, *i.e.,* searching-based models and representation learning-based models. Specifically, searching-based models aim to infer the missing facts by retrieving the logic chains which matched with predefined ones in the given KGs. For example, we can easily get the relations between A and C is *uncle of* by matching the logic chain *(A, father of, B)*$\bigwedge$*(B, cousin of, C)*. In this category, how to achieve (1) efficient path searching, and (2) effective rule matching are two key problems, where multiple models are developed based, such as DeepPath [16], STAR [17], etc. However, these models suffer from poor scalability due to the hard rule matching. Thus, more recent models are developed based on representation learning techniques, such as TransE [1], MKGformer [2], etc. These models learn the embedding based on existing facts and then rank top k candidate facts based on the likelihood calculated by scoring functions, where the 1^{st} candidate fact corresponds to the predicted fact.

Although existing representation learning models achieve promising performances, the structural information, as the important characteristic between KGs and traditional knowledge bases, should be better leveraged, thus leading to better reasoning performance and more complete KGs. Actually, some models [6, 14] have made some progress toward it, but there are still spaces to be explored. To fill the gap, we first comprehensively review the existing works for knowledge graph reasoning, and then observe four structural attributes in KGs, *i.e.,* two for basic static KGs, and two for temporal and multi-modal KGs, and propose four models based on them. Beyond my current research scope, I find that there are two key problems restricting the development of KGR, *i.e.,* efficiency, and the way to cooperate with LLMs, which I plan to work on in the future. In summary, the contribution of our PhD thesis consists of the following five main parts.

(1) We comprehensively review 211 existing KGR models and 69 typical datasets for three aspects, *i.e.,* techniques, scenarios, and graph types.
(2) We observe the relational symmetrical structures underlying the KGs and design a contrastive learning strategy based on it to enhance the discriminative capacity of different KGE backbones.
(3) We leverage the structure information underlying the homogeneous view of the KG and the neighbour-enhanced subgraph to improve the expressive ability of GraIL-based models.
(4) We observe the similarity within the KG structures around periodic events, and design periodic and relational correspondence units to leverage such information sufficiently for temporal KGR.
(5) We better leverage the graph structure with two simple yet effective strategies, *i.e.,* weighted summation and alignment constraint, for multi-modal KGR, rather than just treating it as a retrieval map for matching attributes in different modalities of the same entity.

2 LANDMARKS

My PhD thesis targets the research on representation learning for KGR by designing effective mechanisms to better utilize the information underlying the graph structures in KGs. Specifically, five landmarks are reached as shown in Fig. 2, *i.e.,* (1) comprehensive survey [9], (2) a new static transductive KGR model (KGE-SymCL [7]), (2) a new static inductive KGR model (MINES [10]), (3) a new temporal KGR model (RPC [8]), and (5) a new multi-modal KGR model (SGMPT [11]). We breify describe the main idea of these works, and more details can be found in the corresponding papers.

2.1 Comprehensive Survey for KGR

Before working on KGR, we first conduct a comprehensive review of it. Although there are several survey papers [3, 4, 19, 20], most of them only focus on static KGR but omit the recent progress in other KGs, *i.e.,* temporal KGs and multi-modal KGs. Besides, the review criterion mainly relies on the techniques of different KGR models but ignores reasoning scenarios and graph types, which are useful for new researchers to quickly select the KGR model suitable for their own research scenarios or application scenarios. Besides, in order to help new researchers like me better understand the typical and latest KGR models, we conducted a more comprehensive survey for KGR, tracing from static to temporal and then to multi-modal KGs. Specifically, a bi-level taxonomy is designed, *i.e.,* top level (graph types) and base level (techniques and scenarios). In particular, we carefully discuss reasoning scenarios for the reviewed models, *i.e.,* transductive and inductive scenario for static KGR, and interpolation and extrapolation scenario for temporal KGR. Moreover, the performances, as well as datasets, are summarized and presented. Moreover, we point out the challenges and potential

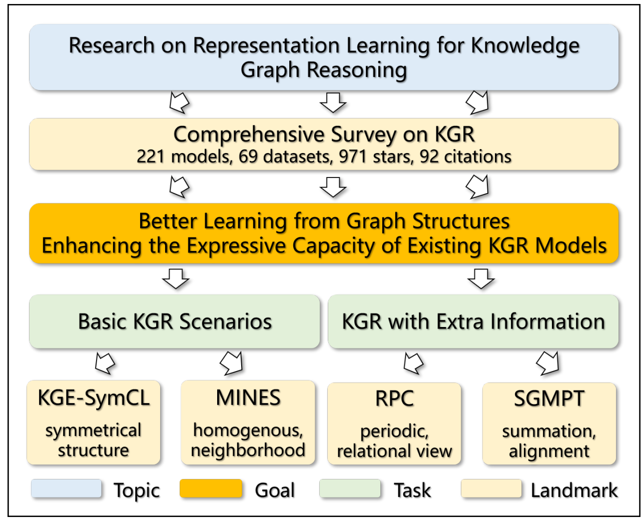

Figure 2: The framework of my research.

opportunities to enlighten the readers. The corresponding open-source repository is shared on GitHub [1] and the corresponding paper is referred as [9].

2.2 Basic KGR Scenario

2.2.1 KGE-SymCL. Knowledge graph embedding (KGE) aims at learning powerful representations to benefit various artificial intelligence applications. Meanwhile, contrastive learning has been widely leveraged in graph learning as an effective mechanism to enhance the discriminative capacity of the learned representations. However, the complex structures of KG make it hard to construct appropriate contrastive pairs. Only a few attempts [13, 15] have integrated contrastive learning strategies with KGE. But, most of them rely on language models (*e.g.,* Bert) for contrastive pair construction instead of fully mining information underlying the graph structure, hindering expressive ability.

Surprisingly, we find that the entities within a relational symmetrical structure are usually similar and correlated. Concretely, neighbors are usually treated to have similar semantics in existing homogeneous graph contrastive learning methods, which benefits the positive contrastive pair construction. However, it is not suitable for knowledge graphs as shown in Fig. 3 (b). Moreover, we assume that such semantic similarity underlying the neighborhood structures in homogeneous graphs is actually caused by the symmetrical positions of the neighbors. Inspired by it, we observe that the relation-symmetrical structure, which can be commonly found in KGs, will also bring a similar property. This specific structure information will be a good criterion for contrastive KGE. Specifically, entities located in relation-symmetrical positions are usually similar and correlated, and this property can be utilized to construct contrastive positive pairs. For example, the *Bob* and *Jones* are relation-symmetrical about *Basketball* in Fig. 3 (c), which reveals the similar semantics between *Bob* and *Jones* (i.e., both playing basketball). The observed property is overlooked by the existing contrastive KGE models, thus leading to sub-optimal performance.

[1] https://github.com/LIANGKE23/Awesome-Knowledge-Graph-Reasoning

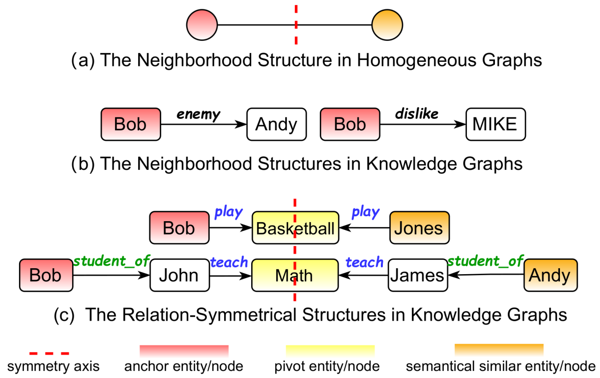

Figure 3: Illustration of neighborhood and relation-symmetrical structures, where relationships are symmetrical. Sub-Fig. (a) and (b) show the differences between neighborhood structures in homogeneous graphs and KGs. The semantics of neighbors may be opposite in KGs, while they are assumed to be similar inhomogeneous graphs. Sub-Fig. (c) shows symmetrical entities in relation-symmetrical structures will be similar in KGs. More details can be found in [7].

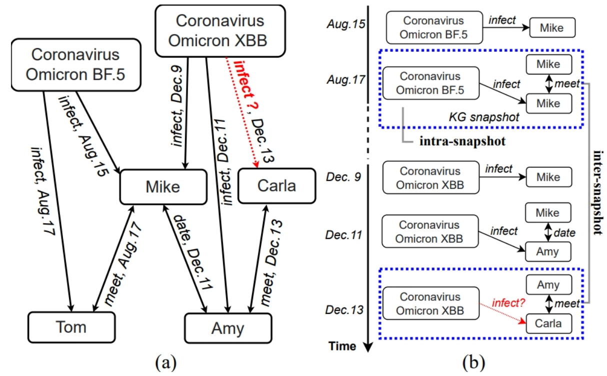

Figure 4: Illustration of temporal knowledge graph reasoning (TKGR) [8]. Sub-graphs (a) and (b) are two different views of the TKGs. By mining the logical patterns underlying the TKGs, TKGR models aim to infer the missing event, which is represented in red dotted edges. Besides, blue boxes indicate different KG snapshots and two gray lines demonstrate that "intra-" and "inter-" are used to describe the interactions "within" and "between" snapshots, respectively.

Thus, a knowledge graph contrastive learning framework is proposed by [7], termed KGE-SymCL, which mines symmetrical structure information in KGs to enhance the discriminative ability of KGE models. Concretely, a plug-and-play approach is proposed by taking entities in the relation-symmetrical positions as positive pairs. Besides, a self-supervised alignment loss is designed to pull together positive pairs. Experimental results show that KGE-SymCL can be easily adopted to various KGE models for performance improvements. More details can be found in paper [7].

2.2.2 MINES. Typically, there are two reasoning settings [9, 14] in static KGR, including transductive setting and inductive setting. Typically, in the transductive scenario, entities in test graphs are all seen in the model during training. In contrast, inductive relation reasoning for knowledge graphs, aiming to infer missing links between brand-new entities, has drawn increasing attention. The models developed based on Graph Inductive Learning, called GraIL-based models, have shown promising potential for this task. However, the uni-directional message-passing mechanism hinders such models from exploiting hidden mutual relations between entities in directed graphs. Besides, the enclosing subgraph extraction in most GraIL-based models restricts the model from extracting enough discriminative information for reasoning. Consequently, the expressive ability of these models is limited.

To address the problems, a novel GraIL-based inductive relation reasoning model, termed MINES, is proposed in [10] by introducing a Message Intercommunication mechanism on the Neighbor-Enhanced Subgraph. Concretely, the message intercommunication mechanism is designed to capture the omitted hidden mutual information. It introduces bi-directed information interactions between connected entities by inserting an undirected/bi-directed GCN layer between uni-directed RGCN layers. Moreover, inspired by the success of involving more neighbors in other graph-based tasks, we extend the neighborhood area beyond the enclosing subgraph to enhance the information collection for inductive relation reasoning. Extensive experiments on twelve inductive benchmark datasets demonstrate that our MINES outperforms existing state-of-the-art models, and show the effectiveness of our intercommunication mechanism and reasoning on the neighbor-enhanced subgraph. More details can be found in paper [10].

2.3 KGR with Extra Information

2.3.1 RPC. Reasoning on temporal knowledge graphs (TKGR), aiming to infer missing events along the timeline, has been widely studied to alleviate incompleteness issues in TKG, which is composed of a series of KG snapshots at different timestamps. Two types of information, *i.e.,* intra-snapshot structural information and inter-snapshot temporal interactions, mainly contribute to the learned representations for reasoning in previous models, as shown in Fig. 4. However, these models fail to leverage (1) semantic correlations between relationships for the former information and (2) the periodic temporal patterns along the timeline for the latter one. Thus, such insufficient mining manners hinder expressive ability, leading to sub-optimal performances.

To address these limitations, a novel reasoning model, termed RPC, is proposed by [8] which sufficiently mines the information underlying the Relational correlations and Periodic patterns via two novel Correspondence units, *i.e.,* relational correspondence unit (RCU) and periodic correspondence unit (PCU). Concretely, relational graph convolutional network (RGCN) and RCU are used to encode the intra-snapshot graph structural information for entities and relations, respectively. Besides, the gated recurrent units (GRU) and PCU are designed separately for sequential and periodic inter-snapshot temporal interactions. Moreover, the model-agnostic time vectors are generated by time2vector encoders to guide the time-dependent decoder for fact scoring. Extensive experiments on six benchmark datasets show that RPC outperforms the state-of-the-art TKGR models, and also demonstrate the effectiveness of two novel strategies in our model.

2.3.2 *SGMPT.*

Multimodal knowledge graphs (MKGs), which intuitively organize information in various modalities, can benefit multiple practical downstream tasks, such as recommendation systems, and visual question answering. However, most MKGs are still far from complete, which motivates the flourishing of MKG reasoning models. Recently, with the development of general artificial architectures, the pretrained transformer models have drawn increasing attention, especially for multimodal scenarios. However, the research of multimodal pretrained transformer (MPT) for knowledge graph reasoning (KGR) is still in its early stages. As the biggest difference between MKG and other multimodal data, the rich structural information underlying the MKG still cannot be fully leveraged in existing MPT models. Most of them only utilize the graph structure as a retrieval map for matching images and texts connected with the same entity. This manner hinders their reasoning performances.

To this end, a graph Structure Guided Multimodal Pretrained Transformer is proposed by [11] for knowledge graph reasoning, termed SGMPT. Specifically, the graph structure encoder is adopted for structural feature encoding. Then, a structure-guided fusion module with two different strategies, *i.e.,* weighted summation and alignment constraint, is first designed to inject the structural information into both the textual and visual features. To the best of our knowledge, SGMPT is the first MPT model for multimodal KGR, which mines the structural information underlying the knowledge graph. Extensive experiments on different datasets demonstrate that our SGMPT outperforms existing state-of-the-art models and prove the effectiveness of the designed strategies.

3 FUTURE WORKS

Beyond my current research scope, there are two key problems restricting the development of KGR, *i.e.,* efficiency, and the way to cooperate with LLMs, which I plan to work on in the future.

Efficient KGR. Existing KGR models require either full graph propagation or full graph searching, which is hard to scale to real-world scenarios, since billion-node-level graphs. To alleviate such issues and make the existing models better benefit our real-world applications, we plan to try to filter out the key entities in given KGs by using techniques like graph pooling, subgraph extraction, etc. Therefore, the scale of KGR models can be smaller, leading to a more efficient algorithm.

Collaborative Reasoning with KGs and LLMs. Large language models (LLMs), *i.e.,* ChatGPT, GPT-4, have huge impacts due to their promising reasoning capacity and generalizability. However, these models still suffer from their poor reliability, which may be solved when well cooperated with KGR models, like using knowledge graph-based retrieval augmented generation (KG-RAG) techniques. Moreover, leveraging KGs to constrain the hallucination problem in LLMs is also worth exploring.

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