Graphical Abstract

Improving Embedded Knowledge Graph Multi-hop Question Answering by introducing Relational Chain Reasoning

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Highlights

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• Our model takes advantage of the knowledge graph embedding technique, and this help capture implicit KG relational information.

• To the best of our knowledge, our proposed model is the first to consider the question relational direction and order information by utilizing the Siamese network.

• Our model is trained with weak supervision by predicting the intermediate relational chain to perform the multi-hop KGQA task, this help improve the accuracy of the model without increasing the training data.
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Abstract

Knowledge Graph Question Answering (KGQA) aims to answer user questions from a knowledge graph (KG) via identifying the reasoning relations between topic entity and answer. As a complex branch task of KGQA, multi-hop KGQA requires reasoning over multi-hop relational chain preserved in KG to arrive at the right answer. Despite of successes made in recent years, the existing works on answering multi-hop complex question are faced with the following challenges: i) Suffering from misunderstanding of user’s intentions due to the neglect of explicit relational chain order reflected in user question. ii) Incorrectly capturing relational types on weak supervision of which dataset lacks of intermediate reasoning chain annotations due to expensive labeling cost. iii) Failing to consider implicit relations between the topic entity and the answer implied in structured KG because of limited neighborhood size constraint in subgraph retrieval based algorithms. To address these issues in multi-hop KGQA, we propose a novel model in this paper, namely Relational Chain based Embedded KGQA (Rce-KGQA), which simultaneously utilizes the explicit relational chain described in natural language question and the implicit relational chain stored in structured KG. Our extensive empirical study on two open-domain benchmarks proves that our method significantly outperforms the state-of-the-art counterparts like GraftNet, PullNet and EmbedKGQA. Comprehensive ablation experiments also verify the effectiveness of our method on the multi-hop KGQA task. We have made our model’s source code available at github: https://github.com/albert-jin/Rce-KGQA.

Keywords:
Question Answering, Knowledge Graph based Multi-hop QA, Neural Semantic Parsing, Knowledge Graph Embedding
1. Introduction

Knowledge Base Question Answering (KBQA) Xiao et al. (2019b) is an attractive service mining and analytics method which has attracted extensive attention from academic and industrial circles in recent years. Given a natural language question, the KBQA system aims to answer the correct target entities from a given knowledge base (KB) Bin et al. (2020). It relies on certain capabilities including capturing rich semantic information to understand natural language questions clearly and seek correct answers in large scale structured knowledge databases accurately. Knowledge Graph Question Answering (KGQA) Hao et al. (2017); Michael and Luke (2018) is a popular research branch of KBQA which uses a knowledge graph (KG) as its knowledge source Bin et al. (2020); Yunshi et al. (2021) and uses factoid triples stored in KG to answer natural language questions. Thanks to KG’s unique data structure and its efficient querying capability, users can benefit from a more efficient acquisition of the substantial and valuable KG knowledge, and gain excellent customer experience.

Early works Lan et al. (2019); Yunshi et al. (2019) on KGQA focus on answering a simple question, where only a single relation between the topic entity and the answer are involved. For example, in the question “What films did [Martin Lawrence] act in?”, as depicted in Fig.1, there only exists a single relation ‘starred_actors’ between the topic entity ‘Martin Lawrence’ and the answer. The final answer only relies on just a single KG fact (Martin Lawrence, starred_actors_reverse, Black Knight). To solve simple question tasks, most traditional methods Bast and Haussmann (2015); Abujabal et al. (2017) create diverse predefined manual templates and then utilize these templates to map unstructured questions into structured logical forms. Unfortunately, these predefined templates and hand-crafted syntactic rules are both labor-intensive and expensive. Moreover, these approaches require crowd workers to be familiar with linguistic and specific domain expert knowledge. Due to the dependency on large-scale fixed rules and manual templates, these methods cannot handle complex questions which require multiple relations inferences.

To make KGQA more applicable in realistic application scenarios, researchers have shifted their attentions from simple questions to complex questions. Knowledge graph multi-hop question answering is a challenging task which aims to seek answers which are multiple hops away from the topic entity in the knowledge graph. For example, the question “Who directed the films which [Martin Lawrence] acted in?” is a complex multi-hop question which requires a relational chain (starred_actors, directed_by) which has multiple relationships to arrive at the corresponding answers. This task is a relatively complex task compared with its simple counterparts due to the multi-hop relations retrieval procedure Yunshi et al. (2021) which requires more
than one KG fact in the inference.

Previous approaches Dong et al. (2015); Jonathan et al. (2013); Haitian et al. (2019); Yunqi et al. (2020); Yu et al. (2020b,a) for handling complex question answering construct a specialized pipeline consisting of multiple semantic parsing and knowledge graph answer retrieving modules to complete the KGQA task. However, they mostly have several drawbacks and encounter various challenges. We summarize these challenges as follows:

![Diagram of Freebase subgraph](image)

Figure 1: The Freebase subgraph entered on the topic entity [Martin Lawrence] of the example questions. The red, yellow, green, green with an imaginary line, and grey circles denote the topic, intermediate, expected, unexpected and irrelevant entity nodes, respectively. The green, red and grey colored edges indicate the correct, incorrect and irrelevant reasoning chains, respectively.

**Unexpected Relation Type Recognition.** As the first step of KGQA, a semantic parser of most existing methods suffers from low accuracy in recognizing the correct relational type implied in questions, which hinders downstream answering reasoning. For example, as shown in Fig.1, let us consider questions where the topic entity and answer are connected by a multiple-hop reasoning chain, e.g., “Who acted in the movies directed by the director [Martin Lawrence]?” To answer this type of question, the related two facts (Martin Lawrence, directed_by_reverse) and (A Tine Line, starred_actors_reverse, Gone Fishin) help derive the answers within the neighborhood of the topic entity [Martin Lawrence]. Typically, these methods
are prone to encounter incorrect relational reasoning \((AB \rightarrow AC)\) when we mistake the unexpected relational chain \((\text{starred}_\text{actors}_\text{reverse}, \text{written}_\text{by})\) for the expected relational chain \((\text{starred}_\text{actors}_\text{reverse}, \text{directed}_\text{by}_\text{reverse})\). Thus, it is necessary to optimize relational semantics parsing for more accurate user intention recognition.

**Unexpected Relation Order Recognition.** Semantic parsing-based Boris (2000); Gao et al. (2021) methods mostly do not effectively utilize the correlation information of relationship order and direction from user question expression. They become more susceptible to incorrect question understanding when the questions are complicated from both semantic and syntactic aspects. The accuracy rate of parsing syntactics can be dramatically decreased by those with long-distance dependency. More especially, tracing back to the above question example and Fig.1, in addition to the correct chain (with green arrows), the spurious multi-hop chain (with red arrows) from entity node [Martin Lawrence] to [Kim Bass] can lead to incorrect reasoning results when the semantic parser module fails to parse semantics such as reversing \((AB \rightarrow BA)\) or shuffling \((ABC \rightarrow BCA)\) the correct order of the relational chain. In short, we need to accurately capture longer ordered relational mappings implied in user language expressions to reach correct answers.

![Figure 2: A structured knowledge graph related to the user question “Who is [Renate Remedio]’s cousin?”](image)

The illustration typically introduces implicit relations between the topic entity and the answer that hide in KG.

**Implicit Relation Reasoning & Subgraph Neighborhood Constraint.**
Most mainstream KGQA methods Huang et al. (2018); Molino et al. (2016) cannot implicitly capture knowledge of implicit relational chains for reasoning due to the limited neighborhood size constraint. All the answers are provided by retrieving the extracted question subgraph. Let us consider the question “Who is Renate Remedio’s cousin?” As depicted in Fig.2, the corresponding knowledge graph has no direct relational chain between the topic entity Renate Remedio and answer Amaranta Orsule. In other words, for successive KGQA solutions in the future, it is important to have the capability to discover the implicit factoid knowledge (Remedio ← Cousin → Orsule) in the incomplete KG by the explicit relational chain (Remedio ← Father - Siblings - Mother → Orsule), similar to the KG-based link prediction task Deepak et al. (2019). Furthermore, most existing methods suffer from the undesirable constraint of answer detection from a pre-specified localized KG sub-graph neighborhood. For example, the state-of-the-art (SOTA) method GraftNet Haitian et al. (2018) whose answer is restricted to be subset of the entities present in localized KG sub-graph neighborhood, only reports a recall around 0.55 on an incomplete KG where only half of the original triples are presented.

To alleviate these limitations and challenges for the multi-hop KGQA task, in this paper, we introduce a novel architecture, namely Relational Chain based Embedded KGQA, which supports the integration to learn the explicit relational mappings implied in the user’s expression and the implicit knowledge from the structured KG, similar to link prediction. Our proposed approach solves these limitations by simultaneously utilizing the explicit semantic relational chain described in the question and the implicit relational chain between the structured KG nodes. We use the knowledge graph embedding and construct the Answer Filtering Module to calculate the mutual relationship between the topic entity and answer. Motivated by the previous work EmbedKGQA Saxena et al. (2020), our model leverages an end-to-end neural network that utilizes the KG entity and relation embeddings to provide complex questions answers from the KG. Since our model replaces the traditional pipeline procedure of generating and retrieving a localized subgraph at intermediate reasoning steps, it helps to decrease memory costs efficiently and obtain computational efficiency. To obtain a more competitive performance in large-scale KG, we apply an extra reasoning procedure called the Relational Chain Reasoning Module to prune the candidate entities ranked by the Answer Filtering Module. We apply a Siamese architecture Mueller and Thyagarajan (2016) based on the long short-term memory (LSTM) and transformer RoBERTa Yinhan et al. (2019) to learn the semantic similarity between the relational chain of the problem description and the KG factoid relational chain. It also leverages the external supervised signal of the relational chain from the training sample. By calculating the semantic similarity
between question semantics and candidate entity retrieval chain, we can further determine the final answer more accurately. The internal construction details of our model are introduced in Sec. 4.

We summarize the contributions of this paper as follows:

1. We propose a novel approach namely Relational Chain based Embedded KGQA which includes two main modules: the Answer Filtering Module and the Relational Chain Reasoning Module. Different from previous studies, our model simultaneously takes advantage of the knowledge graph embedding and training with weak supervision by predicting the intermediate relational chain implied in KG to perform the multi-hop KGQA task.

2. We introduce the Answer Filtering Module, a knowledge graph embedding based end-to-end network for preliminary answer filtering. This module can address the incompleteness problem brought by the missing links in the incomplete knowledge graph thanks to its capability of capturing implicit KG relationships. Furthermore, we consider all entities as candidate answers in this step, so our model won’t suffer from the out-of-reach issues brought by limited subgraph neighborhood constraint.

3. Our proposed Relational Chain Reasoning Module can help capture the multi-hop relations surrounding the topic node to support the results more accurately. We apply the Siamese network Mueller and Thyagarajan (2016) to calculate the vector representation-based semantic similarity score between the user’s question and KG structured knowledge. To the best of our knowledge, our proposed sub-module is the first to consider the question relational direction and order information by utilizing the Siamese network.

4. Our experimental results on two widely adopted KGQA benchmarks show that our method significantly outperforms the recent SOTA methods (average 1.2% absolute improvement across hit@1 evaluation metric). Furthermore, using an extensive ablation study, we demonstrate the superiority and effectiveness of our proposed model for the multi-hop KGQA task.

The rest of the paper is organized as follows. We first provide a thorough review of the related KGQA works in Sec. 2. Next, we introduce the preliminary knowledge about the KGQA task in Sec. 3. Following the internal structure of our model, we then explicate our two features: Answer Filtering Module in Sec. 4.2 and Relational Chain Reasoning Module in Sec. 4.3, respectively. Sec. 5 describes the experimental details on two open-domain datasets. Finally, in Sec. 6, we conclude our contributions in this work and suggest several promising innovations for our Relational Chain based Embedded KGQA in the future.
2. Related Work

Our work is closely related to the Multi-hop Knowledge Graph Question Answering, Knowledge Graph Embedding, Siamese Network, and Pretrained Language Model.

2.1. Multi-hop KGQA

Multi-hop Knowledge Base Question Answering includes two mainstream branches: Information Retrieval-based (IR) and Semantic Parsing-based (SP-based). The most popular methods fall into these two categories.

2.1.1. Semantic Parsing Methods

SP-based approaches follow a parse-then-execute procedure. These methods LAN and Jing (2020); He et al. (2021); Xiao et al. (2019a); Saxena et al. (2020); Chen et al. (2021) can be summarized into the following steps: (1) question semantic understanding: parsing relations and subjects involved in complex questions, (2) logical formula construction: decode the subgraph into an executable logic form such as high-level programming languages or structured queries such as SPARQL, (3) KG-based positioning and querying: search from KGs using the query language and provide query results as the final answer. Owing to its intermediate procedure of generating expressive logic forms, SP-based methods are more interpretable than IR-based methods counterparts. Nonetheless, for most existing SP-based methods, more relations in complex questions indicate a larger search space of potential logic forms for parsing, which will dramatically increase the computational cost.

Yu et al. Mo et al. (2017) pointed out that KG relation detection is a core component and entity linking is a key step in KGQA tasks. To improve the recognition accuracy of both two subtasks, they proposed the Hierarchical Residual BiLSTM (HR-BiLSTM) to encode question descriptions and word-level and phrase-level relationship path. The new HR-BiLSTM module calculates the similarity scores for all the questions and textual relationships, which integrates these two components entity linking and relationship path identification into a single step and enhances each other. When in inference, the model only selects the highly-scored (relations, topic entity) pairs as correct answers from candidates.

Miller et al. Alexander et al. (2019) proposed a ideal domain specific KGQA framework, named Key Value-Memory networks (KV-MemNN), which was proved to be effective to support answer reasoning over specific domain multi-source knowledges like textual documents and structured KB. It performs QA by utilizing a widely used long-term memory mechanism to reason on a key-value structured memory network. They defined three operations, i.e., key hashing, the model first fetchs all KB triples
relevant to given questions and then stores their topic entities and relationships in
the key slot, tail entity in the value slot; key addressing, the model assigns each
memory unit with a normalized relevance weight by the dot product operation as
the relevance probability between the question and each key representations in the
memory; value reading, the model reads the values of all addressed memories by
taking their weighted sums of all values and relevance weights, and use the outputs
to represent intermediate reasoning results, which is then used to update the question
representation. To obtain the final prediction over all candidate answers, the model
repeats the key addressing and value reading steps in the Ranking component several
times.

However, the KV-MemNN obviously exists the following challenges: 1) It of-
ten fails to precisely update multi-relation question queries during multiple memory
reading. 2) It reads the memory repeatedly since they can not well determine when
to stop. 3) It focuses more on memory facts understanding rather than the properly
questions understanding, so it does not perform as well as expected when applied
to the scenario where its questions are complicated and associated with complex
constraints, such as open-domain KGQA task. 4) It selects the candidate with the
highest similarity score as the only answer in default, so it conducts inefficiently
when the questions contain more than one answer.

To solve these challenges mentioned above, Xu et al. Kun et al. (2019) proposed
an interpretable mechanism to enable basic KV-MemNN model to work for com-
plex questions, which yielded the state-of-the-art performances on two benchmarks.
Enhanced KV-MemNN was introduced a novel STOP strategy into multi-hop mem-
ory reading to generate flexible number of queries and was introduced a new query
updating method, which considers the already-addressed keys in previous hops as
well as the value representations that avoids repeated or invalid memory readings.
For multi-constraint questions, the model takes value representation of each hop
into consideration by accumulating all the value representations of both current and
previous hops to address each relevant constraints at different hops.

2.1.2. Information Retrieval Methods

IR-based approaches typically include a series of procedures as follows: question-
specific graph extraction, question semantics representation, extracted graph-based
reasoning and answer candidates ranking. Given a complex question description,
these methods Zi-Yuan et al. (2019); Jain (2016) first construct a question-specific
subgraph which includes all question-related entity nodes and relation edges from
KGs without generating an executable logic formula, then employ a question repre-
sentation module to encode user question tokens as low-dimensional vectors. Sec-
ondly, An extracted-graph based reasoning module conducts a semantic matching algorithm to aggregate the center entity’ neighborhoods information from the question-specific subgraph. At the end of the reasoning, they rank all the entities’ scores in the subgraph by utilizing an answer ranking module and predict the top-ranked entities as the final answers. Based on feature representation technology, IR-based approaches can be divided into feature engineering-based approaches and representation learning-based approaches.

*IR-based* feature engineering approaches Yao and Van (2014) rely on manually defined and extracted features, which are time-consuming and can not detect the whole question semantics. To solve these problems, representation learning *IR-based* methods convert questions and related entities into distributed vector representations in the same dimension space and treat KGQA tasks as semantic matching between distributed representations of questions and candidate answers Bin et al. (2020).

Sun et al. Haitian et al. (2018) proposed a integrated framework namely *GRAFT-Net*, which is adopted an knowledge fusion strategy, where the answers are selected from a heterogeneous question-specific subgraph constructed from the KG and textual documents based on the given questions. The subgraph contains three factors: entity nodes, sentence nodes and a special type of edges which indicates the mutual relations between entity and sentence nodes. During answer detection, the convolution neural network GRAFT-Net spreads central entity node feature to neighboring nodes in several iterations and determines whether an entity node is answer or not.

However, the automatically constructed subgraph in GRAFT-Net relies heavily on heuristic rules and may lead to serious error cascading and bring incorrect reasoning. Thus, soon after the GRAFT-Net Haitian et al. (2018) proposed, Sun et al. Haitian et al. (2019) proposed a learned iterative process for topic-entity-centric graph construction. The improved method, called *Pull-Net*, where the “pull” classifier is weakly supervised that only utilizes QA pairs for supervision. It first selects seed entity nodes by GRAFT-Net and a novel classification model at each iteration step. Then, more and more extra valuable entities and sentences are introduced into the current graph through several pre-defined operation iterations and the final answer can be determined by the same procedure as GRAFT-Net Haitian et al. (2018). Experimentally PullNet improves dramatically over the prior state-of-the-art methods Haitian et al. (2018); Jain (2016); Yao and Van (2014) even under weakly supervised signals and incomplete KGs.

Besides these tradition subgraph generation methods, researchers also try to incorporate the KG embedding mechanism as extra information into entity and relation representations to alleviate the incomplete KG sparsity problems. Inspired by relationship completion and missing link prediction tasks in the KGs, Saxena et
Saxena et al. (2020) proposed a novel framework, named EmbedKGQA, which leverages the pre-trained KG embeddings to enrich the learned entity and relation representations. Extensive comparative experiments on multiple benchmarks show that EmbedKGQA is particularly effective in performing multi-hop KGQA over sparse KGs.

2.2. Knowledge Graph Embedding

Knowledge Graph Embedding Xiao et al. (2019a) is to embed a KG’s factoid triples knowing all entities and relations into continuous and low-dimensional embedding representation space, such that the original entities and relations are well preserved in the vectors. Representative KG embedding models exploit the distance-based scoring function \( f(\cdot) \) which is used to measure the plausibility of a triple \((\text{topic entity, predicate, and tail entity})\) as the distance between the head and tail entity such as TransE A.Bordes et al. (2013) and its extensions (e.g. TransH Wang et al. (2014)), DistMult Min-Chul et al. (2015) and ComplEx Trouillon et al. (2016). In short, a typical KG embedding technique generally consists of three steps: (1) representing entities and relations, (2) defining a scoring function, and (3) learning entity and relation representations. Thanks to its ability to simplify the manipulation while preserving the KG inherent structure, it can benefit a variety of downstream tasks to take the entire KG into consideration, such as entity alignment Sun et al. (2020), relation prediction Deepak et al. (2019) and even KGQA work Saxena et al. (2020). The effectiveness of knowledge graph embedding in various real-world NLP tasks Tingting et al. (2021); Ali et al. (2018) motivates us to explore its potential advantages in the KGQA task.

2.3. Siamese Network

The Siamese network Mueller and Thyagarajan (2016) is a semantic textual similarity metric that is built on top of a feature representation network such as CNN Chopra et al. (2005) and RNN Mueller and Thyagarajan (2016). Given an example input pair, the Siamese network first maps these two inputs into sequences of the word embedding vector using large-scale pretrained embeddings like Glove Jeffrey et al. (2014), then passes these vectors through the feature representation extractor’s forward procedure and get the semantic vector representations, respectively. Finally, the Siamese network applies \( \ell^1 \) norm (Manhattan distance) or \( \ell^2 \) (Euclidean distance) norm as the distance measurement function to calculate the similarity between these two representations. Furthermore, the long short-term memory (LSTM) is superior to the original RNNs for learning long range dependencies because its memory cell units can capture rich features across lengthy language token sequences, thus in this
work, we employ the Siamese adaptation of the bidirectional LSTM network with the goal of learning the semantic relational chain.

2.4. Pretrained Language Model: RoBERTa

Bidirectional Encoder Representations from Transformers Ashish et al. (2017), or BERT, is a revolutionary self-supervised pretraining technique that learns to predict intentionally hidden (masked) sections of text. Crucially, the representations learned by BERT have been shown to generalize well to downstream tasks, and when BERT was first released in 2018 and it achieved state-of-the-art results on many NLP benchmark datasets.

RoBERTa Yinhan et al. (2019), which was proposed by Liu et al., is built on BERT’s language masking strategy and modifies key hyperparameters in BERT, and it can be regarded as a heavily optimized version of BERT. It includes removing BERT’s next-sentence pretraining objective, and trains with much larger mini-batches and learning rates. It was also trained on an order of magnitude more data than BERT, for a longer amount of time. This allows RoBERTa representations to generalize even better to downstream tasks compared to BERT. The improved model RoBERTa achieves state-of-the-art results on GLUE, RACE and SQuAD benchmarks, without multi-task finetuning for GLUE or additional data for SQuAD.

3. Preliminaries

In this section, we formally introduce the preliminary knowledge Yunshi et al. (2021); Bin et al. (2020) on the multi-hop KGQA task formulation and its related definitions. Before the formulaic description, all the summarized pre-defined notations for the KGQA task are given as follows. We denote a KG as $G(\epsilon, \mathcal{R})$ in which $\epsilon$, $\mathcal{R}$ respectively denote the entities and relation set, and we use $(h, \ell, t)$ to represent a factoid triple in KG. We use an uppercase and lowercase letter to denote a matrix (e.g. $W$) and a vector (e.g. $v$). The $\ell^n$ norm of a vector is denoted as $\|p\|_n$.

Definition 1 (Multi-hop question) Saxena et al. (2020); Bin et al. (2020); Yunshi et al. (2021) If a natural language question involves more than one predicate between the topic entity and answer, then we believe the answer is multiple hops away from the topic entity in the KG. Thus, we identify this type of questions as a multi-hop question. For example, let us consider the multi-hop question: “When did the film production company announce which actor also directed the movie [Cast a Deadly Spell]?”’, which consists of several predicates which correspond to the KG relational links: release_year, starred_actors, directed_by respectively.
Definition 2 (Knowledge Graph Embedding) Wang et al. (2017) The KG embedding algorithm Xiao et al. (2019a); Wang et al. (2017) aims to map all the KG components including entity and relation to a low-dimension and continuous vector space. Given a KG consisting of $n$ entities and $m$ relations, we firstly initialize the values of $h$, $\ell$ and $t$ randomly. Then, a scoring function $f_\ell(h, t)$ which we defined measures the relation of a fact triple $(h, \ell, t)$. Finally, the embedding algorithm utilizes a margin-based ranking criterion to optimize the embedding distribution that maximizes the overall plausibility of factoid triples $(h, \ell, t)$ and minimize the plausibility of spurious triples $(h', \ell', t')$ simultaneously.

Definition 3 (Multi-hop KGQA task) Bin et al. (2020); Yunshi et al. (2021) The multi-hop question was introduced in definition 1. In this section, we define a knowledge graph (KG) as $G$. $G$ is a directed graph whose nodes represent entities and edges represent relations, and each triple in the KG represents an atomic realistic fact, such as (Joseph Robinette Biden, president of, USA).

Formally, given a complex natural language question in the format of a sequence of tokens $\mathbf{w} = w_1, w_2, ..., w_l$ and the available KG $G$, the KGQA task first links the topic entity $w_i, ..., w_j$ to the KG $G$. The subject mentioned in a question is also named as a topic entity. Then, it identifies the most possible KG relations which are related to the user’s question. Using these two steps, the goal of KGQA is to determine the factual answer with triples stored in KG, denoted by the set $A_q$, to query $q$ from the candidate entities $E$ by leveraging the topic entity and related relations in KG. Specially, we focus on solving complex question answering, termed the multi-hop KGQA task, where the answer is multiple hops away from the topic entity in knowledge graph, which means these questions require more than one KG triple.

4. Our Proposed Model

Our Relational Chain based Embedded KGQA is a two-stage pipeline model which consists of two components: Answer Filtering Module and Relational Chain Reasoning Module.

4.1. Overview

As illustrated in Fig.3, given a real-world question and an available KG, the Answer Filtering Module first jointly leverages topic entity embedding and question representation to score all possible candidate entities in this KG to provide a set of pruned candidate answers for this question. However, the entity nodes in a KG are often as large as a million scale, hence it could be noisy and inaccurate when
Figure 3: This figure shows our overall pipeline architecture for the multi-hop KGQA task. The green rectangles denote our two sub-modules, the solid arrows and dashed arrows indicate the information flowing through our model and the intermediate results. The next figures [4, 5] also illustrate this by using the typical user’s complex question “Who acted in the movies directed by the director [Martin Lawrence]?”. 

comparing the topic entity with all other entities $t$. To make the learning more efficient and accurate, we do not directly select the top-1 scoring entity from the sorted entities as our final answer. Instead, we introduce the extra module Relational Chain Reasoning Module to take the relation type and order of semantic relational chain into consideration for a higher hit@1 accuracy result.

Before being fed into the next stage, we transform these intermediate candidate entities to their shortest relational chains which point to the question’s topic entity by retrieving them in KG and map these ordered chains to sequences of embedding which corresponds with our embedded KG. The Relational Chain Reasoning Module receives the intermediate results generated by the last step. Then, it simultaneously utilizes the relational chain sequences and user question to measure the mutual similarity score through our Siamese network. Taking the question relational chain reasoning details into consideration can help increase the accuracy of answer prediction compared with the first stage, the Answer Filtering Module. Last, after sorting the scored candidates, we choose the entity which has the highest similarity score as the final answer. Algorithm 1 formally illustrates how our method works
and predicts the final answer for a given multi-hop question, where \( \ell \) denotes the question semantic representation, and \( \phi \) denotes the ComplEx scorer, respectively.

**Algorithm 1** Stepwise Answer Reasoning for RceKGQA

**Require:** Knowledge Graph \( \mathcal{G}(\varepsilon, \mathcal{R}) \); L length Question \( q \), denote \( \{ \mathbf{w}_j \}_{j=1}^{L} \); question topic entity \( h \) in KG;

**Ensure:** Predicted Answer \( e_{\text{ans}} = \arg \max_{t' \in \mathcal{A}} \phi(h, \ell, t') \)

1. Through ComplEx, we obtain KG relation embeddings \( \mathbf{W}_r \) and entity embeddings \( \mathbf{W}_e \) where \( e \in \varepsilon \) and \( r \in \mathcal{R} \).
2. for all \( t' \) such that \( t' \neq h \cap t' \in \varepsilon \) do
3. \( \ell = \text{Attn}(\text{BiLSTM}(\{ \mathbf{w}_j \}_{j=1}^{L})) \)
4. \( \text{Score}(t') = \phi(h, \ell, t') \)
5. end for
6. Select top-N (\( N \in \{5, 10, 15\} \)) scoring tail entities from last step, denotes \( \{t''_i\}_{i=1}^{N} \)
7. for all \( t''_i \in \{t''_i\}_{i=1}^{N} \) do
8. Retrieval its shortest relational chain \( r^*_i = \{r_j\}_{j=1}^{M} \), where \( M \) is the chain length.
9. end for
10. Collect all candidates and its relational chain as a set \( \{[t''_i; r^*_i]\}_{i=1}^{N} \).
11. for all \( [t''_i; r^*_i] \in \{[t''_i; r^*_i]\}_{i=1}^{N} \) do
12. \( \mathcal{V}_q = \text{fc2} \circ \text{dropout}(\text{relu}(\text{fc1}(\text{RoBERTa}(\{ \mathbf{w}_j \}_{j=1}^{L})))) \)
13. \( \mathcal{V}_{r^*_i} = \text{Attn}(\text{BiLSTM}(r^*_i)) \)
14. \( \text{Score}(\mathcal{V}_q, \mathcal{V}_{r^*_i}) = \exp \left( - \| \mathcal{V}_q^{(2)} - \mathcal{V}_{r^*_i}^{(2)} \|_2 \right) \)
15. end for
16. Select the highest scoring entity \( \arg \max_{t''_i} \text{Score}(\mathcal{V}_q, \mathcal{V}_{r^*_i}) \) from \( \{[t''_i; r^*_i]\}_{i=1}^{N} \), denote as \( e_{\text{ans}} \).

### 4.2. Answer Filtering Module

As the first step of our model, our Answer Filtering Module aims to filter an entity set from all KG entities as candidate answers via three steps. These three operational steps are illustrated in Fig.4. The three steps respectively relate to three sub-modules: Graph Embedding Generator, Question Semantic Parser and Answer Scorer. We introduce each sub-module followed by the system processing order.

#### 4.2.1. Graph Embedding Generator

Traditional solutions could not handle many scenario problems such as Implicit Relation Reasoning and Subgraph neighborhood Constraint. Inspired by the competitive performance of previous work EmbedKGQA Saxena et al. (2020), we observe
that the global relation knowledge and structure information preserved in KG embedding could be potentially used to solve these issues efficiently and improve the overall question answering accuracy.

In this work, our used KG is also embedded in continuous low-dimensional vector space to obtain all sparse representations for all entities and relations existed in KG so as to simplify computations on the KG. We apply the Complex Embeddings (ComplEx) Trouillon et al. (2016) approach to embed relations and entities in complex vector space. Compared with traditional KG embedding methods like TransE A.Bordes et al. (2013) and its extensions, semantic matching models such as Holographic Embeddings Nickel et al. (2016), ComplEx and RESCAL M et al. (2011) have shown that they can generally yield better results. All KG embeddings are initialized randomly from uniform distributions. Generally, the hyper-parameters about entity and relation embedding dimension are not less than 100 and in this paper we set embedding dimension at 200 which follows previous similar works.

In each training steps, positive facts which present correct real-world relational triples are sampled from all factoid triples existing in KG. Negative facts which present fake factoid relational triples are generated from negative sampling in negative example generation step, where it randomly replaces the tail entity with an incorrect entity or replaces the relation with incorrect relation.

Considering about the samples count ratio of positive to negative ones, Trouillon et al. Trouillon et al. (2016) further investigated the influence of different number of negative samples for each positive one. Their work demonstrates that generating more negatives usually lead to better performance, and around fifty negatives per positive example is an appropriate trade-off between reasoning accuracy and training cost, so our implementations also follow this prior setting.

Given \( h, t \in \varepsilon \) and \( \ell \in \mathcal{R} \), this embedding approach would provide \( v_h, v_{\ell}, v_t \in \mathbb{C}^d \) for each relation triple \((h', \ell', t')\), and the scoring function is defined as follows:

\[
\phi(h', \ell', t') = \text{Re} \left( \langle v_h, v_{\ell}, \bar{v}_t \rangle \right)
\]

\[
= \text{Re} \left( \sum_{k=1}^{d} v_h^{(k)} v_{\ell}^{(k)} \bar{v}_t^{(k)} \right)
\]

\[
\phi(h', \ell', t') > 0 \quad \forall a \in \mathcal{A} \quad (1)
\]

\[
\phi(h', \bar{\ell}', \bar{t}') < 0 \quad \forall \phi(h', \bar{\ell}', \bar{t}') \notin \mathcal{A} \quad (3)
\]

where the \( \text{Re}(\cdot) \) means taking the real part of a complex value, the \( \bar{v}_t \) denotes the conjugate of \( v_t \), the \( \bar{\ell}', \bar{t}' \) is the random replaced wrong relation and wrong tail.
entity of the $\ell', t'$, and the $\mathcal{A}$ means the set including all real-world knowledge triples.

Optimization Eq.1 aims to minimize the values for all false triples less than 0, Eq.3 and maximizes the values for all true triples greater than 0, Eq.2. It can be easily carried out by stochastic gradient descent (SGD) or Adam optimizer at each training iteration. Lastly, the original structure and relation information in the KG are preserved in these learned vectors, which helps complete the downstream procedures efficiently.

4.2.2. Question Semantic Parser

In this part, we introduce the Question Semantic Parser, which consists of a recurrent neural network (bidirectional-LSTM) and extra self-attention operation, to help represent the question’s meanings. During the inference procedure, the Question Semantic Parser takes a question as the input and then provides a predicted vector $\hat{\ell}$ as this question’s relationship representation between the topic and answer in KG.

As shown in Fig.4, we build this sub-module based on the hierarchical neural network. Firstly, we encode the $L$ length question $\{t_j\}$, for $j = 1, \ldots L$ into a sequence of word embedding vectors $\{v_j\}$ through our word embedding layer whose parameters are learnable during the training procedure. The word embedding dimension is consistent with the recurrent network’s hidden dimension. Then we employ a single
layer bidirectional LSTM to learn a forward hidden state sequence \((\hat{h}_1, \hat{h}_2, \ldots, \hat{h}_L)\) and a backward hidden state sequence \((\hat{h}_1, \hat{h}_2, \ldots, \hat{h}_L)\). Compared to general RNN, bidirectional LSTM is a special RNN which mainly solves the gradient disappearance and gradient explosion challenges and captures better long-distance semantics during long sequence modeling. Our LSTM component uses 256 as its dimension of hidden representations \(h_t\) and memory cells \(c_t\). It is well known that the performance of LSTMs depends crucially on their initialization and offers a strong starting point to facilitate model convergence, so we initialize our bidirectional LSTM weights with Xavier Glorot and Bengio (2010) initialization which is markedly superior to other initialization methods such as Gaussian, Uniform and Kaiming initialization He et al. (2015).

Taking the forward step as an example, the next state \(\hat{h}_j\) based on last state \(\hat{h}_{j-1}\) is computed via the following operations.

\[
f_j = \sigma \left( W_{xf}x_j + W_{h\hat{h}}\hat{h}_{j-1} + b_f \right) \tag{4}
\]

\[
i_j = \sigma \left( W_{xi}x_j + W_{hi}\hat{h}_{j-1} + b_i \right) \tag{5}
\]

\[
o_j = \sigma \left( W_{xo}x_j + W_{ho}\hat{h}_{j-1} + b_o \right) \tag{6}
\]

\[
c_j = f_j \odot c_{j-1} + i_j \tanh \left( W_{xc}x_j + W_{hc}\hat{h}_{j-1} + b_c \right) \tag{7}
\]

\[
\hat{h}_j = o_j \odot \tanh \left( c_j \right) \tag{8}
\]

The variables \(f_j, i_j, o_j\) in the above equations are the input, forget and output gate’s activation vectors respectively, where \(\odot\) is the cell state vector, \(= \sigma\) and \(\tanh\) are the hyperbolic tangent and sigmoid functions. After the information flows through LSTM, we concatenate the forward \(\hat{h}_j\) and backward \(\hat{h}_j\) and obtain the combined features \(h_j = [\hat{h}_j; \hat{h}_j]\).

Different word tokens make different contributions to the relationship semantic recognition, for example, words which are prepositions and articles are more irrelevant for discovering question semantics than relational demonstrators. Thus, after LSTM we apply the self-attention mechanism to capture more valuable features. The attention operation details are shown in Eq.9 and Eq.10, given a LSTM hidden representation, a full connect layer, activation function \(\tanh\) and softmax operation.
jointly generate the attention weight $\alpha_j$ at first. Then, as shown in Eq.10, the final attention vector representation $s_j$ which is the semantic representation of the language question are aggregated by the weighted sum operation of $h_j$ and $a_j$.

$$\alpha_j = \frac{\exp(a_j)}{\sum_{i=1}^{L} \exp(a_i)} \quad \text{where} \quad a_j = \tanh(w^\top_a[h_j] + b) \quad (9)$$

$$s_j = \sum_i \alpha_{ij} h_{ij} \quad (10)$$

All the weight matrices, weight vector $W$, and bias terms are calculated based on the training data, i.e. LSTM gate unit weight matrix $\{W_f, W_i, W_o\}$ and attention weight matrix $w^\top_a$. In this way, we obtain the rich relationship semantics implied in natural language questions for answer reasoning.

### 4.2.3. Answer Scorer

Similar to the ComplEx Trouillon et al. (2016) scoring function which depicted in Eqs. 1, 2 and 3, as shown in Eq.11, we learn a answer ranker $\text{Rank}(t)$ for each candidates $t$, namely Answer Scorer to score the (topic entity, relationship semantic) pair against all possible KG entities $t \in \varepsilon$ by maximizing the probabilities of positive samples $t \in A$ and minimizing the negative sample $t' \notin A$, where the $A$ means the set including all real-world knowledge triples.

$$\text{Rank}(t) = \left\{ \begin{array}{ll}
\max(\phi(h, k, t)), & \forall t \in A \\
\min(\phi(h, k, t')), & \forall t' \notin A
\end{array} \right. \quad (11)$$

Since our Question Semantic Parser is designed to fit realistic relationship features, all the pretrained KG entity embeddings are frozen during the model convergence procedure.

Instead of simply selecting the entity with the highest score due to its low accuracy but high recall performance, we conduct a rough filtering by select top-n, where $n \in \{5, 10, 15\}$ to obtain the intermediate scored candidate entities that have a high answer recall rate. For the inference, the Answer Scoring Module gives each candidate a plausibility score to indicate its answer confidence and filter out the top-n scored intermediate result which is fed into the next step, the Relational Chain Reasoning module.

### 4.3. Relational Chain Reasoning Module

Our available KG often contains a large number of entities and has enormous factoid triples, and it could be inaccurate when comparing all candidate embedding
representations against with each other. Specifically, after training the Answer Filtering Module, we obtain all the scored entities for each training sample. During the prediction result analysis, we observe that the model performance on hit@5 outperforms that on hit@1 metric, which could be due to the influence of a large number of noisy entities number in the large-scale KG. Furthermore, since the answer is given as the only ground-truth information, a major challenge for multi-hop KGQA is that it usually lacks intermediate reasoning supervision signals.

To tackle these issues, we propose an extra component for our KGQA work, termed the Relational Chain Reasoning Module. As the final and important step of our approach, it aims to improve the reasoning accuracy through considering the reasoning chain order and its relational type under weak supervised situation. Its training procedure is irrelevant to the Answer Filtering Module, but its training dataset is constructed from the Answer Filtering Module’s prediction results.

Formally, we use the trained Answer Filtering Module to obtain the sorted scored entities \(\{[e_{it}; s_{it}]\}_{i=1}^n\), \(\{[e_{it}; s_{it}]\}_{i=1}^n\) and \(\{[e_{ie}; s_{ie}]\}_{i=1}^n\) for the training, validating, and testing datasets, respectively. Then, these scored results are truncated by only reserving top-\(n\) \((n \in \{5, 10, 15\})\) candidates. Next, for the rough filtered results in each experimental sample, if it belongs to the correct answers, we construct a cor-

Figure 5: Structure of the designed Relational Chain Reasoning Module.

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responding positive sample \([q; \{r\}_{i=1}^c]\), in which \(q\) denotes the question tokens and \(\{r\}_{i=1}^c\) is the \(c\) length shortest path searched by the graph retrieval algorithm, and so do the negative samples that are not inside in the correct answers.

4.3.1. Siamese Network Based Similarity Scoring

As shown in Fig.5, we introduce our novel sub-module Siamese Network Based Similarity Scoring, which is essentially a Siamese network Mueller and Thyagarajan (2016). The module’s two feature detectors aim to extract the question Eq.12 and the relational chain semantic representations Eq.13. They are constructed by a pretrained transformer RoBERTa Yinhan et al. (2019) to generate question vector \(V_q\) from question \(q = \{w_i\}_{i=1}^N\) and a single-layer bidirectional LSTM to generate relational chain vector \(V_r\) from relational chain \(r^* = \{r_j\}_{j=1}^M\). RoBERTa is a revolutionary self-supervised pretraining technique that learns to predict intentionally hidden sections of language text. Moreover, the representations learned by RoBERTa has been shown to generalize even better to many NLP downstream tasks compared to original BERT Ashish et al. (2017). Structure details will be described in the next successive two subsection. After informations passes through these two encoded networks, the semantic feature similarities Eq14 in the vector representation space are subsequently used to infer the semantic similarity between the question and relational chain from the topic entity to answer.

\[
V_q = W_2^T(drop(W_1^T(RoBERTa(q)) + b_1)) + b_2
\] (12)

\[
V_r = Attn(BiLSTM(r^*))
\] (13)

\[
Score(V_q, V_r) = \exp\left(-\|V_q^{(2)} - V_r^{(2)}\|_2\right)
\] (14)

Here, we explain why we use a semantic similarity score between relation chain \(V_r\) and question representations \(V_q\) to determine the right answer in detail. Taking the above question “Who acted in the movies directed by the director [Martin Lawrence]?” as an example, we denote the natural language tokens as \(q\), and we firmly believe that the implied question semantic is similar and its representation is closer to the relational chain representation in vector space, “\(directed_by_reverse \rightarrow starred_actors_reverse\)”, which is correct in both order and type. It is inconsistent and far away from the relational chains which have the wrong type or order, such as “\(starred_actors_reverse \rightarrow directed_by_reverse\)” and “\(directed_by_reverse \rightarrow written_by_reverse\)”. 

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As shown in Eq.14, we train the similarity scorer using the stochastic gradient descent (SGD) backward propagation algorithm under the mean-squared-error (MSE) loss function. Then we endow our training criterion with the $\ell^2$ (Euclidean distance) norm metric to avoid the model parameter distribution being highly warped. The predicted relatedness labels to lie in $[0, 1]$, for the positive sample we maximize the prediction value as close as possible to 1, and the negative sample as close as possible to 0. Finally, after sorting the scored candidates, we choose the entity which has the highest similarity score as the final answer.

4.3.2. Question Semantic Representation

As depicted in Fig.5 left, we use and finetune a standard version of RoBERTa to obtain the hidden state $V_q$ lying in start token $[CLS]$ for our question encoders. Note that we reformat question $q$ through replacing the topic entity’s mention in the question with a token “NE”. And we respectively supplement two special characters $'[CLS]'$ and $'[SEP]'$ before and after reformatted question, which follows the BERT default configuration. This aforesaid operations can help our model better distinguish the topic entity and other question word mentions. Afterwards, we link the question’s topic entity mention to KG node through matching with standard KG entity literal representations. We regard it as the semantic signal for answer reasoning and then adopt two full connect layers, neuron activation function ReLU Xavier et al. (2011) and a dropout layer to get better feature learning capability. After the above step, a vector representation is generated by the last full-connected layer, and we use the vector to compare space distance similarity with the output of another feature encoder, Relational Chain Representation module.

4.3.3. Relational Chain Representation

As depicted in Fig.5 right, we provide the Relational Chain Representation module which consists of a single layer bidirectional LSTM and a self-attention layer. Given the KG relational chain embedding sequence as input, this module learns and captures the relevant and necessary semantic information for answering reasoning. It has a similar structure to the Question Semantic Parser in the Answer Filtering Module, but the token embeddings used are not initialized by random initialization. Instead, we apply the pretrained KG relation embedded representations existing in Sec 4.2.1 to embed our relational chain.

Formally, as depicted in Eq.13, for relational chain $r^* = \{r_j\}_{j=1}^M$, where $M$ denotes the chain length, each relationship representation $r_j (j = 1, 2, ..., M)$ is initialized with the pretrained KG relational embeddings. Next, we feed the embedded vectors $r^*$ into a single-layer bidirectional LSTM network to obtain a series of output
states $h_1, h_2, ..., h_M$, where the $j$-th relation $h_j$ denotes $[\vec{h}_j; \vec{\bar{h}}_j]$, a combined vector of forward LSTM state output $\vec{h}_j$ and backward LSTM state output $\vec{\bar{h}}_j$. Then the new question representation $q = [h_1, h_2, ..., h_M]$ can be transformed through a self-attention operation, which is similar to Answer filtering Module counterpart, shown in Eq.9, 10. Through the aforesaid forward propagation that is similar to Question Semantic Parser, we can obtain a question semantic vector $V_q$ which has the same dimension as relational chain vector $V_r$ for the following similarity computation step.

5. Experiment

In this section, we evaluate our proposed Rce-KGQA against competitive baselines on two benchmark datasets to investigate whether our model can outperform other methods on reasoning over the weakly supervised signal and incomplete knowledge graph. And we also append extensive ablation experiments and case study to carefully verify and vividly demonstrate that the necessity, superiority and meaning about our ideas in this work. The datasets as well as the pytorch implementation of our model are publicly available at https://github.com/albert-jin/Rce-KGQA.

5.1. Datasets and Evaluation Metric

Here, we first describe the two benchmark datasets we use in this work and then give a brief introduction of the metric hit@1 we used for model evaluation.

**MetaQA** Yuyu et al. (2018) is a large KGQA dataset which provides an original version Vanilla and two variations. In this paper, we use the original ones because it is designed manually. This dataset includes up to 75w QA pairs which are merely 2-hop questions. The questions’ literal description are generated by cross-language translation, English→French→English. It relies on a large-scale movie domain which contains 9 relationship types, 43234 entities and up to 135k factoid triples.

**WebQuestionsSP-tiny** Wentau et al. (2016) dataset is a relatively small dataset with a total of 4736 QA pairs. This QA dataset’s available KG is a subset of Freebase that contains all the facts that are within 2-hops of any entity mentioned in the questions of the original WebQuestionsSP, which have more than 188w entities and 1000 relationship types. Following Saxena et al. (2020), for all topic entities labeled in the original Freebase, we construct subgraph containing other KG entities close to them by the PageRank-Nibble algorithm (PRN) Reid et al. (2006). In this way, theoretically, the pruned KG is likely to contain the corresponding answer entity for nearly whole questions.

Metric hit@1 is a standard assessment for measuring the ratio in all validation samples that the highest scored entity belongs to the correct answers. In brief, if the
Table 1: Statistics for dataset MetaQA and WebQuestionsSP-tiny. MetaQA contains three subsets of different complex question relational chain length, 1/2/3 hop MetaQA, but WebQuestionsSP-tiny does not.

|                | Train  | Dev   | Test  |
|----------------|--------|-------|-------|
| MetaQA 1-hop   | 208970 | 19947 | 9992  |
| MetaQA 2-hop   | 231844 | 14872 | 14872 |
| MetaQA 3-hop   | 227060 | 14274 | 14274 |
| WebQSP-tiny    | 2848   | 250   | 1639  |

QA system provides the user with a single entity and this entity is right, we then determine that this prediction is correct. This evaluating indicator is popular and publicly recognized and it has been used in many recent KGQA works Saxena et al. (2020); Zi-Yuan et al. (2019); LAN and Jing (2020).

5.2. Experiment Setting

As we know, hyperparameter choices have a significant impact on the model’s final performance. Our optimal model hyperparameter configuration is summarized as follows. All the LSTM modules we used as feature encoders have a single layer with hidden dimension 256. All the dropout layers randomly drop about 30% of features for inputs during the training step but they do not drop any features during testing. We apply Xavier initialization to initialize each network layer’s training parameters in our model. Our applied pretrained transformer RoBERTa is a base configuration which consists of 12 layers, 768-d hidden size and 12 attention heads for efficient training and inference. The answer filtering module is trained for up to 200 epochs with a batch size of 128 and the relational chain reasoning module is trained for up to 120 epochs with a batch size of 32 on two benchmarks. For every 10 training epochs, we adopt the early-stopping strategy by evaluating hit@1 on the test set to avoid overfitting. During model convergence, the stochastic gradient descent (SGD) optimizer with initial learning rate \( lr = 1e-5 \) is adopted. We used different random seeds to independently validate our best configured model 5 times and report the average validation performances of our model in the next sections.

5.3. Compared Methods

In our experiment, the state-of-the-art methods for comparison are described as follows:
EmbedKGQA Saxena et al. (2020) is a KG embedding driving method for multi-hop KGQA which matches the pretrained entity embeddings with question embeddings generated from the transformer.

SRN Yunqi et al. (2020) is an RL-based multi-hop question answering model which conducts the QA task by extending the inference chains on KG.

KVMem Alexander et al. (2019) The Key-Value Memory Network first attempts to conduct QA over incomplete KGs by augmenting it with text. It utilizes a memory table which stores the KG facts encoded into key-value pairs to retrieve a question-specific subgraph for reasoning.

GraftNet Haitian et al. (2018) is a question description-based semantic subgraph driving method which uses a variational graph CNN to perform QA tasks over question-specific subgraphs containing KG facts, entities and discourses from textual corpora.

PullNet Haitian et al. (2019) improves GraftNet on the retrieval subgraph by introducing the graph retrieval module which utilizes shortest path from the topic entity to answer as the additional supervised signal.

5.4. Main Results

In this section, we compare our model with the state-of-the-art baseline methods on two benchmarks, and the following questions are answered:

Q1. How effective and accurate is the performance of our model compared with other SOTA models?

Q2. Can our model really identify the implicit relations and the indirect linked answer when there is no direct relational chain from topic entity to answer?

5.4.1. Answer Reasoning on MetaQA

As illustrated in Table 2, the overall experimental results on the MetaQA test set clearly demonstrate that our proposed KGQA architecture significantly outperforms state-of-the-art methods on hit@1 metric. Specifically, according to the result of our model’s result on 1-hop MetaQA (identical to WikiMovies), compared to the other methods, Row 1 ~5, we observe that our method’s hit@1 accuracy achieves much high performance up to 98.3%, which is an increase of 1.3% compared to GraftNet Haitian et al. (2018) and PullNet Haitian et al. (2019) and an increase of 0.8% compared to EmbedKGQA Saxena et al. (2020).

For the evaluation of multi-relation questions which require at least two hops of inference to find the answers, hit@1 results on 2-hop and 3-hop MetaQA also achieve
better performance than all other competitive state-of-the-art baselines. Although our model test results on 2-hop not achieve best score, it is also comparable to other SOTA models. It is worth noting that the retrieval-and-reason process of PullNet, which can simultaneously extract answer from both corpora and KGs, is good at reasoning answers over large-scale KGs such as MetaQA. In contrast, we can see that our model Rce-KGQA, which takes relation chain reasoning into consideration, does not drop significantly but almost remains unchanged when the relational chain hop increases. We think the reason may be that the baseline models only consider the question shadow semantic representations, and inevitably introduce noise and incorrect retrieving path over KG. On the other hand, since our model focuses on relational chain order and relation type, it is less sensitive to the hop size and robustness on complex multi-constraint queries over KG. In summary, these results have shown their effectiveness and superiority when considering the question semantic and its relational chain into reasoning, which largely improves the KGQA performance.

| Model       | 1-hop MetaQA | 2-hop MetaQA | 3-hop MetaQA |
|-------------|--------------|--------------|--------------|
| EmbedKGQA   | 97.5         | 98.8         | 94.8         |
| SRN         | 97.0         | 95.1         | 75.2         |
| KVMem       | 96.2         | 82.7         | 48.9         |
| GraftNet    | 97.0         | 94.8         | 77.7         |
| PullNet     |              | 99.9         | 91.4         |
| **Our Model** | **98.3**     | **99.7**     | **97.9**     |

Table 2: Experimental results on three subsets of MetaQA. The first group of results was taken from papers on recent methods. The values are reported using hits@1. The number in bold and underlined number denote the best and second best methods, respectively. This figure corresponds to Sec. 5.4.1.

5.4.2. Answer Reasoning on WebQuestionsSP-tiny

WebQuestionsSP-tiny is a relatively small dataset for training but relies on a large-scale KG (Freebase) whose entities’ count is greater than 10 million. Table 3 presents the evaluation results on the WebQuestionsSP-tiny test set, from which we can observe that our KGQA system still performs better that its other state-of-the-art counterparts. EmbedKGQA (has 3.8% lower hists-at-one than our model) and PullNet (has 2.3% lower hists-at-one than our model).

Specifically, the last row shows that our full model achieves accuracy of up to 70.4% hit@1, which improves a large margin to other prior models. A possible explanation is that the filtering model equips the extra relational chain module with
better reasoning perception, leveraging KG and question implicit features more efficiently, and emphasizing the order of relational triples selection to help our model make a correct decision. Even in large-scale KG along with a small training dataset situations like WebQuestionsSP-tiny, our Rce-KGQA system can still be robust and helpful for handling realistic QA applications.

| Model       | WebQuestionsSP-tiny hit@1 |
|-------------|--------------------------|
| EmbedKGQA   | 66.6                     |
| SRN         | -                        |
| KVMem       | 46.7                     |
| GraftNet    | 66.4                     |
| PullNet     | 68.1                     |
| Our Model   | **70.4**                 |

Table 3: Experiment results compared with SOTA methods on WebQuestionsSP-tiny test set. All QA pairs in WebQuestionsSP-tiny are 2-hop relational questions. The best score is in **bold** and the second-best score is underlined.

5.5. Answer Reasoning for implicit relationship discovery

As shown in Table 4, we verify our method’s ability to discover missing implicit relationships through comparison experiments. The KG which MetaQA uses has no missing link during the reasoning path because the QA question pairs are constructed upon this KG. However, to make it become a realistic setting, we simulate an incomplete KG by randomly removing half (with probability = 0.5) of the factoid triples from it. We call this pruned setting **half** and we call the full KG setting **full** in the text.

The experiments show our method’s implicit relation discovering capability substantially outperforms other state-of-the-art methods over incomplete KG. The amount of improvement is significant, with an increase of 43.7% compared to KVMem in hit@1. Furthermore, our competitive model also delivers an average 1.7% hit@1 rate on 2-hop MetaQA half setting and performs well on 3-hop MetaQA half setting while PullNet still achieves highest hit@1 score.

Hence many baseline methods such as GraftNet, PullNet require constructed question-specific subgraph, therefore they are lack of capability to recall the answer nodes out of their generated subgraph and can not perform well in real QA scenarios. Fortunately our model, which utilizes the KG link prediction properties, does not limit its capability to this constraint. Although those complex questions in WebQuestionsSP-tiny could be easily covered by hand-crafted rules as many did, our
model is not suitable enough for such predefined rules. We think it is crucial to use more advanced reasoning capabilities to correctly enhance our model \textit{Rce-KGQA}, which we leave for future work.

| Models      | 2-hop MetaQA | 3-hop MetaQA |
|-------------|--------------|--------------|
|             | full         | half         | full         | half         |
| KVMem       | 82.7         | 48.4         | 48.9         | 37.6         |
| GraftNet    | 94.8         | 69.5         | 77.7         | 66.4         |
| PullNet     | \textbf{99.9} | 90.4         | 91.4         | \textbf{85.2} |
| EmbedKGQA   | 98.8         | 91.8         | 94.8         | 70.3         |
| Our Model   | \textbf{99.7} | \textbf{92.1} | \textbf{97.9} | 84.7         |

Table 4: Experimental results about reasoning on incomplete KG (hit@1 as a percentage). We consider two different KG settings, \textbf{full} and \textbf{half}. \textbf{Full} denotes the complete KG and \textbf{half} denotes a KG subset whose 50% factoid triples are randomly removed.

5.6. Answer Filtering Result Analysis

To further examine whether our proposed enhancement to the extra module \textit{Relational Chain Reasoning Module} ia an advanced and obvious improvements, we analyse the reasoning performance of first module \textit{Answer Filtering Module} and put the answer distributions with prediction in Table 5. In Table 5, as we can see that if we regard the scored candidate entities provided by this module as the final answer, the hit@1 accuracy rate drops a lot compared to hit@5 and hit@10. This observation indicates that the model which does not consider relational chain order and relation type achieves very poor performance and proves the necessity and superiority of our proposed module, the \textit{Relational Chain Reasoning Module}.

Furthermore, from Table 5, we can clearly observe that almost right answers of our used datasets collectively distribute in the top-5 of our model’s predictions. Due to this high recall rate of our first module, the \textit{Answer Filtering Module}, we think we can only rely on a few top-scoring candidates (such as top-15, top-10, or even top-5) to further filter the final answer more accurately. So during our model training and inference experiments, we tried several experimental schemes and we consider the number of top-scoring candidates, specifically, how to select candidates to automatically generate positive or negative samples and how to cut the top-N candidates for the sub-module \textit{Relational Chain Reasoning Module} inference. The related experimental details are shown in Sec. 5.6.
Table 5: Our Answer Filtering Module answer reasoning performance on three different metrics hit@1, 5, 10. Model performance on Hit@5 and Hit@10 accuracy highly outperform which on Hit@1 accuracy.

| Dataset         | Hit@1_r | Hit@5_r | Hit@10_r |
|-----------------|---------|---------|----------|
| 2-hop MetaQA    | 0.861   | 0.995   | 0.999    |
| 3-hop MetaQA    | 0.858   | 0.984   | 0.997    |

5.7. Candidates Filtering Strategy Analysis

Our QA solution Rce-KGQA is a complex pipeline system, and we inevitably have to choose some crucial hyper-parameters to require optimal model, these predefined parameters include full connected/LSTM layer number, dropout rate, learning rate, and so on. As illustrated in Sec. 5.6 and Table 5, different selection modes about top-scoring candidates during training and inference have a huge impact of the final model performances. We now further investigate what influence would happened to our model in different candidates selection mode.

Firstly, from Table 5 we can observe that our first step ‘answering filtering’ consistently achieve high recall performances on hit@5. Now we manually choose and cut difference sorted candidate answers and conduct our comparison experiments. Specifically, from Sec. 4.3 we know that the dataset for Relational Chain Reasoning Module training is dynamically constructed by the last step. And the data construction follows the selection of top-N sorted scoring entities in which number N simultaneously decides the proportion of positive/negative samples and the intermediate results selection during inference step. For example question Q, during model evaluation, we firstly obtain the intermediate scoring candidate answers \{[A_i; S_i]\}_{i=1}^N. In next step, we should use the Relational Chain Reasoning Module provides all filtered candidates with a more precise score to get final answer. Selecting how many top scoring entities to conduct the further step exactly becomes our focus research point.

We choose four strategies which include top-{5, 10, 15, 20}, then from the corresponding experiments we receive the following results which is shown in Table 6. From experimental comparison results we clearly find that in top-5 selection strategy, our model achieves the highest hit@1 performances and achieves the second highest performances in top-10 strategy, in both 2-hop MetaQA and 3-hop MetaQA datasets. These phenomena may come from two aspects. First, the recall rate of the module Relational Chain Reasoning Module is good enough for the next fine-grained screening and the positive/negative samples proportion should be in a suitable extent. Besides, more candidates in model inference step could bring more noise entities which could affect model answer judgment and decrease the overall model performances.
Table 6: Our model final performance statistics about impacts of the four selection strategies: choose top-5, choose top-10, choose top-15 and choose top-20. The values reported are hit@1. Bold and underline fonts denote the best and the second best selection strategies.

| Policy       | top-5 pick | top-10 pick | top-15 pick | top-20 pick |
|--------------|------------|-------------|-------------|-------------|
| 2-hop MetaQA | 0.997      | 0.994       | 0.989       | 0.985       |
| 3-hop MetaQA | **0.979**  | **0.971**   | **0.967**   | **0.967**   |

5.8. Ablation Study

To better understand and gain a deep insight into our model design, we also perform ablation experiments to systematically investigate the impact and contributions of different components. \text{RceKGQA}_r, \text{RceKGQA}_a and \text{RceKGQA}_b are variants of our full model RceKGQA. Note that for our ablated experiments, we remove one component each time. Here we briefly introduce these variants for the ablated experiments.

- \text{RceKGQA}_r removes the Relational Chain Reasoning module and the highest scoring entity is provided by the Answer Filtering Module as the final answer.
- \text{RceKGQA}_a removes all the self-attention operations from the model.
- \text{RceKGQA}_b replaces RoBERTa with LSTM in the question semantic representation part of the Relational Chain Reasoning module.
- \text{RceKGQA} is the full model introduced in this paper.

In this section, the following questions are answered:

**Q1.** How much does the Relational Chain Reasoning Module help for our model’s reasoning accuracy?

**Q2.** Can the attention mechanism really help increase our model’s overall performance?

**Q3.** Is the effectiveness of our method due to the use of RoBERTa in the Relational Chain Reasoning module?

According to the result comparison between RceKGQA and its variant RceKGQA—r, we can clearly conclude that removing the Relational Chain Reasoning Module from the proposed model has a huge impact on the results.

The performance gap between RceKGQA—r which is shown in Row 2 and our full model shown in Row 1 indicates that the semantic relational chain factor plays a pivotal role in answer reasoning, which incorporates relational chain order and relationship type to provide more accurate answers for the terminal user.
As shown in Row 3, when our full model is compared with RceKGQA\(_{-a}\), we can see an average 3.5% performance drop across the hit@1 metric if the self-attention components are removed, which demonstrates the importance of the self-attention mechanism used in our method, as it effectively helps with the final answer prediction. A possible reason is that the self-attention mechanism can distinguish the most relevant and interesting signals from noise information, and help our model better understand the question and relational chain semantic.

RceKGQA\(_{-b}\), which is shown in Row 4, only loses 1.6% hit@1 accuracy compared with our full model, which replaces RoBERTa with BiLSTM, and demonstrates that the usage of the transformer is not a major factor in increasing the overall model performance.

The above ablated statistics confirm that all three components introduced for handling the multi-hop relation question answering contribute to the overall model performance.

| Model        | 1-hop MetaQA | 2-hop MetaQA | 3-hop MetaQA |
|--------------|--------------|--------------|--------------|
| RceKGQA      | 98.3         | 99.7         | 97.9         |
| RceKGQA\(_{-r}\) | 85.8         | 86.1         | 84.8         |
| RceKGQA\(_{-a}\) | 96.1         | 95.9         | 93.4         |
| RceKGQA\(_{-b}\) | 95.9         | 98.2         | 95.6         |

Table 7: Ablation study statistical results for RceKGQA and its three variants (Hit@1 by percentage). Compared with our full model, suffix\(_{-r}\) denotes RceKGQA whose Relational Chain Reasoning module is removed, suffix\(_{-a}\) denotes the RceKGQA variant whose attention operation is dropped and suffix\(_{-b}\) denotes the RceKGQA variant whose question encoder RoBERTa is replaced with BiLSTM.

5.9. Case Study

The major novelty of our approach lies in the introduced relational chain reasoning network. Next, we present a case study to demonstrate how it helps the overall model architecture.

Given a question “In which years were movies released which starred actors who appeared in the movie [Thunderbolt]?”, the right reasoning relational chain preserved in KG is Thunderbolt(movie)-starred_actors_reverse → Stanley Holloway(actor)-starred_actors → The Way Ahead(movie)-release_year → ‘1986’(year). When ignoring the relational chain feature factor and only using the high scored entity generated by the Answer Filtering Module as the final answer, the network mistakes and selects a wrong reasoning path Thunderbolt(movie)-release_year → ‘1991’(year) for the aforesaid question with a very high probability of 0.96 as the answer. Its
attention only focuses on the relationship: release_year, which ignores the repeated relations of starred_actors and starred_actors_reverse. In comparison, the complete model which considers the relational chain factor and utilizes the relational chain reasoning network for fine-grained selection can easily and correctly provide the right answer ‘1986’(year) with a high probability of 0.99 from KG.

This example shows that our relational chain reasoning network indeed provides very useful supervision signals of relational chain recognition at intermediate steps to improve our model’s overall QA performance.

6. Conclusion and Future Perspective

In this work, we introduce an elaborate KG embedding based pipeline approach for the multi-hop KGQA task, termed Relational Chain-based Embedded KGQA. Novel techniques are proposed to effectively utilize QA relational chain parsing to identify the semantics more accurately and leverage the structure information preserved in KG embedding to reason the implicit answer indirectly. Our comprehensive empirical results on two benchmarks demonstrates that our method outperforms many of its state-of-the-art counterparts. The experimental comparison between our approach and its ablated variants also verifies that the proposed model components contribute to the answer reasoning result. We believe KGQA will continue to be an attractive and promising research direction with realistic industrial and domestic scenarios, such as Intelligent Recommendation, Smart Personal Assistant, Big Data Mining Services, and Automatic Customer Services.

In the future, we plan to study the following major problems. (i) To support real-world dynamic application scenarios, the KGQA application is always updated quickly and inevitably accumulates new and immense external knowledge in real time. How can we augment our available KG’s knowledge reserve automatically and incrementally to expand our system’s knowledge coverage? (ii) This model is trained on relatively small QA datasets under weak supervision without external prior knowledge. How can we introduce external knowledge such as knowledge from web pages and other open-domain KGs to improve our question answering system’s performance?

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