

# Toward Subgraph Guided Knowledge Graph Question Generation with Graph Neural Networks

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**Abstract**—Knowledge graph (KG) question generation (QG) aims to generate natural language questions from KGs and target answers. Previous works mostly focus on a simple setting which is to generate questions from a single KG triple. In this work, we focus on a more realistic setting where we aim to generate questions from a KG subgraph and target answers. In addition, most of previous works built on either RNN-based or Transformer-based models to encode a linearized KG subgraph, which totally discards the explicit structure information of a KG subgraph. To address this issue, we propose to apply a bidirectional Graph2Seq model to encode the KG subgraph. Furthermore, we enhance our RNN decoder with node-level copying mechanism to allow directly copying node attributes from the KG subgraph to the output question. Both automatic and human evaluation results demonstrate that our model achieves new state-of-the-art scores, outperforming existing methods by a significant margin on two QG benchmarks. Experimental results also show that our QG model can consistently benefit the Question Answering (QA) task as a mean of data augmentation.

**Index Terms**—Question Generation, Knowledge Graphs, Natural Language Processing, Graph Neural Networks, Deep Learning.

## I. INTRODUCTION

Recent years have seen a surge of interests in Question Generation (QG) in machine learning and natural language processing. The goal of QG is to generate a natural language (NL) question for a given form of data such as text [1], [2], [3], [4], images [5], tables [6], and knowledge graphs (KGs) [7]. In this work, we focus on QG from KGs.

KGs have drawn a large amount of research attention in recent years, partially due to their huge potential for an accessible, natural way of retrieving information without a need for learning complex query languages such as SPARQL. In order to train a large KB question answering (QA) system, a large number of QA pairs are often needed, which can be a severe bottleneck in practice. Developing effective approaches to generate high-quality QA pairs from KGs can significantly address the data scarcity issue for KB-QA.

Motivated by this observation, recent research on KG-QG can be categorized into two classes. The first line of research focuses on generating simple questions from a single KG triple [8], [9], [10]. These models typically apply a Seq2Seq model with copying mechanism for translating either

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a keyword list or a triple into a question. Although these methods produce relatively high-quality questions, they do not necessarily help solve complex multi-hop QA tasks. More recently, [11] presented a multi-hop question generation system named MHQG+AE, which directly works on a KG subgraph and thus is able to generate more complex questions using transformer-based models. However, they still considered a KG subgraph as a set of triples and do not explicitly leverage the intrinsic graph structure.

The task of KG-QG has three unique challenges. The first one is how to learn a good representation of a KG subgraph. A KG subgraph has complex underlying structures such as node attributes, and multi-relation edges. Each node and edge could have (long) associated text comprising multiple words. The second challenge is how to automatically learn a good mapping between a subgraph and a natural language question. How to “copy” some unusual node or edge information that is related to the generated questions. The third challenge is how to effectively leverage the answer information for question generation in KG.

In order to address the above challenges, we present a subgraph guided Knowledge Graph Question Generation approach with Graph Neural Networks (GNNs). To this end, we introduce for the first time the Graph2Seq architecture for the task of KG-QG to address the second challenge. We then extend the regular GNN-based encoder to allow processing directed and multi-relational KG subgraphs to solve the first challenge. We explore two different ways of handling multi-relational graphs. In addition, we propose a simple yet elegant way to leverage the context information from the answers to effectively handle the third challenge. Extensive experimental results demonstrate the superior performance of our proposed model over the state-of-the-art baselines on two benchmarks. Compared to existing state-of-the-art baselines, our model significantly outperforms them by a large margin according to both automatic evaluation and human evaluation.

We highlight our main contributions as follows:

- We propose a novel Graph2Seq model for subgraph guided KG-QG. The proposed Graph2Seq model employs bidirectional graph embedding and we design two different GNN encoders to effectively encode KG subgraphs with directed and multi-relation edges.
- We extend the RNN decoder with a novel copying mechanism that allows the entire node attribute to be borrowed from the input KG subgraph when generating natural language questions.
- We investigate two different ways of initializing node/edge embeddings when applying a GNN encoder to process

KG subgraphs. In addition, we study the impact of directionality (i.e., bidirectional vs. unidirectional) on GNN encoder.

- Experimental results show that our model improves the state-of-the-art BLEU-4 score from 11.57 to 29.40 and from 25.99 to 59.59 on WQ and PQ benchmarks, respectively. A human evaluation study corroborates that the questions generated by our model are more natural (semantically and syntactically) and relevant compared to other baselines. Experiments also show that our QG model can consistently benefit the QA task as a mean of data augmentation.

## II. RELATED WORK

### A. Natural Question Generation from Knowledge Graphs

Early works [12], [13], [7] on QG from KGs mainly focused on template-based approaches that require significant amount of human effort, and have low generalizability and scalability. Recently, Seq2Seq [14], [15] based neural architectures have been applied to this task without resort to manually designed templates and are end-to-end trainable. However, these methods [8], [9], [10] only focus on generating simple questions from a single triple as they typically employ an RNN-based encoder which cannot handle graph-structured data. Very recently, [11] presented a Transformer [16] based encoder-decoder model that allows to encode a KG subgraph and generate multi-hop questions. This is probably the first NN-based method that deals with QG from a KG subgraph instead of just a single triple. However, their method treats a KG subgraph as a set of triples, which does not distinguish between entities and relations while modeling the graph, and also does not utilize explicit connections among triples. Instead of using a Transformer-based encoder which is not designed to utilize graph structure, in this work, we propose to employ a GNN to encode a KG subgraph. To the best of our knowledge, we are the first to introduce the Graph2Seq architecture to the KG-QG task.

There was prior work on applying Graph2Seq models to other kinds of QG tasks. In [3], we proposed a Reinforcement Learning based Graph2Seq model for the task of QG from text. The major difference between this work and our previous work includes, in this work, i) we extend the GNN encoder to handle multi-relational graphs where in [3] edge type information was not modeled, and ii) we extend the word-level copying mechanism in [3] to the node-level copying mechanism.

Our work is also related to prior works on Table2Text which aims to generate text from a table. However, our techniques proposed for KG-QG are very different from the ones used by previous works on Table2Text [6], [17]. Tables are in tabular grid structure whereas KGs can be in arbitrary structure. As a result, almost all existing works on Table2Text relied on RNNs to encode table cell values and column attributes. This is very different from the way that we encode the KG subgraph. We instead rely on GNNs to encode the KG subgraph, which captures both the node/edge features and graph structures.

### B. Graph Neural Networks

Over the past few years, graph neural networks (GNNs) [18], [19], [20], [21], [22], [23], [24], [25], [26] have attracted increasing attention since they extend traditional deep learning approaches to non-euclidean data such as graphs. Given the node feature vectors and the adjacency matrix, GNNs can update all the node embeddings in parallel by incorporating information from neighboring nodes and/or edges. Once the node embeddings are learned, graph-level embeddings can be obtained by applying graph pooling techniques to the node embeddings such as average pooling, max pooling, DiffPool [27] and gPool [28]. GNNs have many successful applications in computer vision [29], [30], [31], [32], natural language processing [33], [34], [35], [36], [37], [38], recommender systems [39], [40], [41], [42], [43], and drug discovery [44], [45], [46], [47], [48], [49], [50]. Because by design GNNs can easily model graph-structured data, recently, a number of works have extended the widely used Seq2Seq architectures [14], [15] to Graph2Seq architectures for various tasks including machine translation [51], [52], semantic parsing [53], and graph-to-text generation (e.g., AMR, SQL and KG to text) [54], [55], [56], [57], [58], [59].

## III. APPROACH

### A. Problem Formulation

Our focus is on natural question generation from a KG subgraph, along with potential target answers; the overall architecture of our approach is shown in Fig. 1. We assume that a KG subgraph is a collection of triples (i.e., subject-predicate-object), that can also be represented as a graph  $\mathcal{G} = (V, E)$ , where  $V \subseteq \mathcal{V}$  denotes a set of entities (i.e., subjects or objects) and  $E \subseteq \mathcal{E}$  denotes all the predicates connecting these entities. We denote by  $\mathcal{V}$  and  $\mathcal{E}$  the complete entity set and predicate set of the KG, respectively. We also assume that all the answers from the target answer set  $V^a$  are from the entity set  $V$ , which is the normal setting of the task of Knowledge Base Question Answering (KBQA) [60]. The task of KG-QG is to generate the best NL question consisting of a sequence of word tokens  $\hat{Y} = \{y_1, y_2, \dots, y_T\}$  which maximizes the conditional likelihood  $\hat{Y} = \arg \max_Y P(Y|\mathcal{G}, V^a)$  where  $T$  is the length of the question. We focus on the problem setting where we have a set of KG subgraphs (and answers) and target questions pairs, to learn the mapping; existing QG approaches [8], [10], [11] make a similar assumption. Although the three main challenges we have discussed before are based on QG from KGs, other QG tasks from other data sources also share some or most of issues when dealing with these tasks. Therefore, our model could be used or adapted to generalize to cope with these tasks as well.

### B. Encoding Layer

Let us denote  $V$  as a set of nodes (i.e., entities)  $\{v_1, v_2, \dots, v_n\}$  in a KG subgraph  $\mathcal{G}$ , where each node is associated with some attributes such as text or ID. Similarly, let us denote  $E$  as a set of edges (i.e., predicates)  $\{e_1, e_2, \dots, e_m\}$  in  $\mathcal{G}$ , where each edge has some initial attributes such as text or ID.

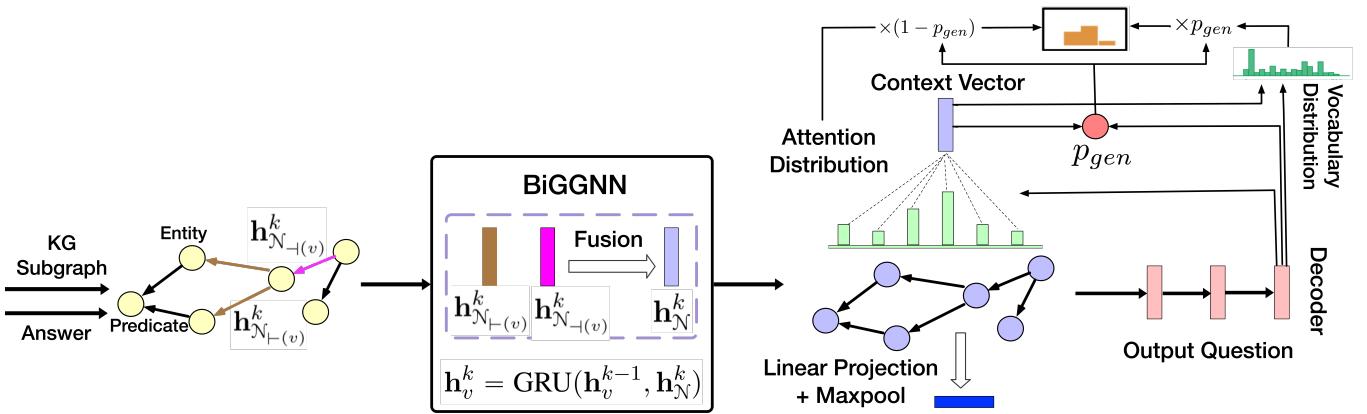


Fig. 1: Overall architecture of our proposed model. Best viewed in color.

1) *Encoding Nodes and Edges*: Before applying the GNN encoder to process a KG subgraph, we need to map nodes and edges to an initial embedding space that encodes their attributes. There are two common ways of encoding nodes and edges in a KG. One solution is based on global KG embeddings that are pretrained on the whole KG by some KG representation learning algorithm such as TransE [61], while the other one is based on pretrained embeddings (e.g., GloVe [62]) of the words making up the textual attributes. In this work, we choose to encode nodes and edges based on word embeddings of their textual attributes in our main model. We posit that it is relatively easier for a model to learn the mapping from the input KG subgraph to the output NL question with both sides based on word embeddings. We empirically compare and analyze the two encoding strategies in our experiments.

In order to encode the nodes and edges in a KG subgraph, we apply two bidirectional LSTMs [63] for nodes (i.e., one for nodes, and one for edges) to encode their associated text. The concatenation of the last forward and backward hidden states of the BiLSTM is used as the initial embeddings for nodes and edges.

2) *Utilizing Target Answers*: In the setting of KBQA [60], [64], it is usually assumed that the answers to a question are entities in a KG subgraph. As a dual task of KBQA, in this QG work, we assume that utilizing the target answers along with the KG subgraph can help generate more relevant questions. To this end, we apply a simple yet effective strategy where we introduce an additional learnable markup vector associated with each node/edge to indicate whether it is an answer or not.

Therefore, the initial vector representation of a node/edge will be the concatenation of the BiLSTM output and the answer markup vector. We denote  $\mathbf{X}^e = \{\mathbf{x}_1^e, \mathbf{x}_2^e, \dots, \mathbf{x}_n^e\}$  and  $\mathbf{X}^p = \{\mathbf{x}_1^p, \mathbf{x}_2^p, \dots, \mathbf{x}_m^p\}$  as the embeddings of the entity nodes and predicate edges, respectively. Both  $\mathbf{X}^e$  and  $\mathbf{X}^p$  have the same embedding dimension  $d$ .

### C. Bidirectional Graph-to-Sequence Generator with Copying Mechanism

While RNNs are good at modeling sequential data, they cannot naturally handle graph-structured data. One might need to linearize a graph to a sequence so as to apply an RNN-

based encoder, which will lose the rich structure information in the graph. Many previous works [51], [52] showed the superiority of GNNs compared to RNNs on modeling graph-structured data. [11] proposed to encode a set of triples via a Transformer [16] by removing positional encoding in the original architecture. Even though a Transformer-based encoder could learn the semantic relations among the triples through the all-to-all attention, the explicit graph structure is totally discarded. In this work, we introduce a bidirectional GNN-based encoder to encode the KG subgraph, and decode the natural language question via an RNN-based decoder equipped with node-level copying mechanism.

1) *Bidirectional Graph Encoder*: Many existing GNNs [19], [22], [65] were not designed to process directed graphs such as a KG. Even though some GNN variants such as GGSNN [23] and MPNN [21] are able to handle directed graphs via message passing across graphs, they do not model the bidirectional information when aggregating information from neighboring nodes for each node. As a result, messages can only be passed across graphs in a unidirectional way.

In this work, we introduce the Bidirectional Gated Graph Neural Network (BiGGNN) which extends GGSNN by learning node embeddings from both incoming and outgoing directions in an interleaved fashion when processing a directed graph. A similar bidirectional approach has been exploited in [54], [66] to extend other GNN variants. While their methods simply learn the node embeddings of each direction independently and concatenates them at the final step, BiGGNN fuses the intermediate node embeddings from both directions at every iteration.

The embedding  $\mathbf{h}_v^0$  for node  $v$  is initialized to  $\mathbf{x}_v$ , namely, a concatenation of the BiLSTM output and the answer markup vector. BiGGNN then performs message passing across the graph for a fixed number of hops, with the same set of network parameters shared at each hop. At each hop of computation, for every node in the graph, we apply an aggregation function that takes as input a set of incoming (or outgoing) neighboring node vectors and outputs a backward (or forward) aggregation vector. In principle, many order-invariant operators such as max or attention [65] can be employed to aggregate neighborhood information. Here we use a simple average aggregator as

follows,

$$\begin{aligned}\mathbf{h}_{\mathcal{N}_{-(v)}}^k &= \text{AVG}(\{\mathbf{h}_v^{k-1}\} \cup \{\mathbf{h}_u^{k-1}, \forall u \in \mathcal{N}_{-(v)}\}) \\ \mathbf{h}_{\mathcal{N}_{(v)}}^k &= \text{AVG}(\{\mathbf{h}_v^{k-1}\} \cup \{\mathbf{h}_u^{k-1}, \forall u \in \mathcal{N}_{(v)}\})\end{aligned}\quad (1)$$

where  $\mathcal{N}_{-(v)}$  and  $\mathcal{N}_{(v)}$  denote the incoming and outgoing neighbors of  $v$ . We then fuse the node embeddings aggregated from both directions,

$$\mathbf{h}_{\mathcal{N}_{(v)}}^k = \text{Fuse}(\mathbf{h}_{\mathcal{N}_{-(v)}}^k, \mathbf{h}_{\mathcal{N}_{(v)}}^k) \quad (2)$$

The fusion function is computed as a gated sum of two information sources,

$$\begin{aligned}\text{Fuse}(\mathbf{a}, \mathbf{b}) &= \mathbf{z} \odot \mathbf{a} + (1 - \mathbf{z}) \odot \mathbf{b} \\ \mathbf{z} &= \sigma(\mathbf{W}_z[\mathbf{a}; \mathbf{b}; \mathbf{a} \odot \mathbf{b}; \mathbf{a} - \mathbf{b}] + \mathbf{b}_z)\end{aligned}\quad (3)$$

where  $\odot$  is the component-wise multiplication,  $\sigma$  is a sigmoid function, and  $\mathbf{z}$  is a gating vector. The gate helps the model to determine how much of the information needs to be reserved from the two aggregated node embeddings.

Finally, a Gated Recurrent Unit (GRU) [15] is used to update the node embeddings by incorporating the aggregation information.

$$\mathbf{h}_v^k = \text{GRU}(\mathbf{h}_v^{k-1}, \mathbf{h}_{\mathcal{N}_{(v)}}^k) \quad (4)$$

After  $n$  hops of GNN computation where  $n$  is a hyperparameter, we obtain the final state embedding  $\mathbf{h}_v^n$  for node  $v$ . To compute the graph-level embedding, we first apply a linear projection to the node embeddings, and then apply max-pooling over all node embeddings to get a  $d$ -dim vector  $\mathbf{h}^g$ .

*2) Handling Multi-relational Graphs:* Knowledge graphs are typically heterogeneous networks that contain a large number of edge types. However, many existing GNNs [19], [22], [23], [65] are not directly applicable to multi-relational graphs. In order to model both node and edge information with GNNs, researchers have extended them by either having separate learnable weights for different edge types or having explicit edge embeddings when performing message passing [21], [67]. While the former solution may have severe scalability issues when handling graphs with a large number of edge types, the later one requires major modifications to existing GNN architectures. In this work, we explore two solutions to adapt GNNs to multi-relational graphs as detailed below.

**Levi graph transformation.** We can directly apply regular GNNs to a multi-relational KG subgraph by converting it to a Levi graph [68]. Specifically, we treat all edges in the original graph as new nodes and add new edges connecting original nodes and new nodes, which results in a bipartite graph. For instance, in a KG subgraph, a triple (Mario\_Siciliano, place\_of\_birth, Rome) will be converted to “Mario\_Siciliano → place\_of\_birth → Rome” where “place\_of\_birth” becomes a new node, and → indicates a new edge connecting an entity and a predicate. Note that since most KG subgraphs are sparse, the number of newly added nodes (and edges as well) will at most be linear to the number of original nodes.

**Gated message passing with edge information.** We also extend BiGGNN to explicitly incorporate edge embeddings when conducting message passing, calling the resultant variant

as BiGGNN<sub>edge</sub>. Specifically, we rewrite the node aggregation function Eq. (1) as follows,

$$\begin{aligned}\mathbf{h}_{\mathcal{N}_{-(v)}}^k &= \text{AVG}(\{\mathbf{h}_v^{k-1}\} \cup \{f([\mathbf{h}_u^{k-1}; \mathbf{e}_{uv}]), \forall u \in \mathcal{N}_{-(v)}\}) \\ \mathbf{h}_{\mathcal{N}_{(v)}}^k &= \text{AVG}(\{\mathbf{h}_v^{k-1}\} \cup \{f([\mathbf{h}_u^{k-1}; \mathbf{e}_{uv}]), \forall u \in \mathcal{N}_{(v)}\})\end{aligned}\quad (5)$$

where  $f$  is a nonlinear function (i.e., linear projection + ReLU [69]) applied to the concatenation of  $\mathbf{h}_u^{k-1}$  and  $\mathbf{e}_{uv}$  which is the embedding of the edge connecting node  $u$  and  $v$ .

*3) RNN Decoder with Node-level Copying:* We adopt an attention-based [70], [71] LSTM decoder that generates the output sequence one word at a time. The decoder takes the graph-level embedding  $\mathbf{h}^g$  followed by two separate fully-connected layers as initial hidden states (i.e.,  $\mathbf{c}_0$  and  $\mathbf{s}_0$ ) and the node embeddings  $\{\mathbf{h}_v^n, \forall v \in \mathcal{G}\}$  as the attention memory. The particular attention mechanism used in our decoder closely follows [72]. Basically, at each decoding step  $t$ , an attention mechanism learns to attend to the most relevant nodes in the input graph, and computes a context vector  $\mathbf{h}_t^*$  based on the current decoding state  $\mathbf{s}_t$  and the attention memory.

We hypothesize that when generating NL questions from a KG subgraph, it is very likely to directly mention (i.e., copy) entity names that are from the input KG subgraph even without rephrasing them. When augmented with copying mechanism [73], [74], most RNN decoders are typically allowed to copy words from the input sequence. We extend the regular word-level copying mechanism to the node-level copying mechanism that allows copying node attributes (i.e., node text) from the input graph. Copying mechanism was used in some previous Graph2Seq papers [57], [75]. The most similar work is [75] which proposed to copy both entities and predicates from the input graph. Unlike [75], we use masked copying mechanism to only copy entity nodes in the transformed Levy graph and do not copy predicate nodes. This is because we assume that for the KG-QG task, it is very likely for humans to directly mention entity names but not necessarily for predicate names that are from the KG.

At each decoding step, the generation probability  $p_{\text{gen}} \in [0, 1]$  is calculated from the context vector  $\mathbf{h}_t^*$ , the decoder state  $\mathbf{s}_t$  and the decoder input  $y_{t-1}$ . Next,  $p_{\text{gen}}$  is used as a soft switch to choose between generating a word from the vocabulary or copying a node attribute from the input graph. We dynamically maintain an extended vocabulary which is the union of the usual vocabulary and all node names appearing in a batch of source examples (i.e., KG subgraphs).

#### D. Training and Testing

As customary for training sequential models, we minimize the following cross-entropy loss,

$$\mathcal{L}_{lm} = \sum_t -\log P(y_t^* | X, y_{<t}^*) \quad (6)$$

where  $y_t^*$  is the word at the  $t$ -th position of the gold output sequence. Scheduled teacher forcing [76] is adopted to alleviate the exposure bias problem. During the testing phase, beam search is applied to generate the output.

Besides training our proposed model with the regular cross-entropy loss, we also explore minimizing a hybrid objective

combining both the cross-entropy loss and Reinforcement Learning (RL) [77] loss that is defined based on evaluation metrics. Most prior works on QG employ cross-entropy based training objective, which is also a de facto choice for training sequential models in many other NLP tasks. However, cross-entropy based training strategy has some known limitations including exposure bias and evaluation discrepancy between training and testing [78], [79], [80]. That is to say, in the training phase, a model has access to the ground-truth previous token when decoding and is optimized toward cross-entropy loss, while in the testing phase, no ground-truth previous token is provided and cross-entropy loss is not used for evaluation. To tackle these issues, we introduce a hybrid objective function combining both cross-entropy loss and Reinforcement Learning (RL) [77] loss for training our Graph2Seq model.

Specifically, we introduce a two-stage training strategy as follows. In the first stage, the regular cross-entropy loss is used,

$$\mathcal{L}_{lm} = \sum_t -\log P(y_t^* | X, y_{<t}^*) \quad (7)$$

where  $y_t^*$  is the word at the  $t$ -th position of the ground-truth output sequence. Scheduled teacher forcing [76] is adopted to alleviate the exposure bias problem. In the second stage, we further fine-tune the model by optimizing a mixed objective function combining both cross-entropy loss and RL loss, defined as,

$$\mathcal{L} = \gamma \mathcal{L}_{rl} + (1 - \gamma) \mathcal{L}_{lm} \quad (8)$$

where  $\gamma$  is a scaling factor controlling the trade-off between the two losses. During the testing phase, beam search is applied to generate the output.

While our architecture is agnostic to the specific RL algorithm, in this work, we employ an efficient yet effective RL approach called self-critical sequence training (SCST) [81] to directly optimize the discrete evaluation metrics. SCST is an efficient REINFORCE algorithm that utilizes the output of its own test-time inference algorithm to normalize the rewards it experiences. At each training iteration, the RL loss is defined by comparing the reward of the sampled output  $Y^s$  with the reward of the baseline output  $\hat{Y}$ ,

$$\mathcal{L}_{rl} = (r(\hat{Y}) - r(Y^s)) \sum_t \log P(y_t^s | X, y_{<t}^s) \quad (9)$$

where  $Y^s$  is produced by multinomial sampling, that is, each word  $y_t^s$  is sampled according to the likelihood  $P(y_t^s | X, y_{<t}^s)$  predicted by the generator, and  $\hat{Y}$  is obtained by greedy search, that is, by maximizing the output probability distribution at each decoding step. As we can see, minimizing the above loss is equivalent to maximizing the likelihood of some sampled output that has a higher reward than the corresponding baseline output.

One of the key factors for RL is to pick the proper reward function. We define  $r(Y)$  as the reward of an output sequence  $Y$ , computed by comparing it to the corresponding ground-truth sequence  $Y^*$  with some reward metric which is a combination of our evaluation metrics (i.e., we used BLEU-4 and ROUGE-L scores in our experiments). This lets us directly optimize the model towards the evaluation metrics.

## IV. EXPERIMENTS

In this section, we conduct extensive experiments to evaluate the effectiveness of our proposed model for the QG task. We also conduct experiments to examine whether our QG model can help the QA task by providing more training data. Besides, we want to examine whether the introduced GNN-based encoder works better than an RNN-based or Transformer-based encoder when encoding a KG subgraph for the QG task. In addition, we explore and analyze two different ways of handling multi-relational graphs with GNNs. Moreover, we empirically compare two different ways of initializing node and edge embeddings before feeding them into a GNN-based encoder. An experimental comparison between bidirectional GNN-based encoder and unidirectional GNN-based encoder is also provided. The code and data is publicly available at <https://github.com/hugochan/Graph2Seq-for-KGQG>.

### A. Baseline Methods

We compare our model against the following baselines: i) L2A [1], ii) Transformer (w/ copy) [16], and iii) MHQG+AE [11]. To the best of our knowledge, MHQG+AE was probably the first NN-based model that focused on QG from a KG subgraph. Their proposed model, called MHQG+AE, employs a Transformer-based encoder [16] to encode a KG subgraph (i.e., a set of triples), and generates an output question with a Transformer-based decoder. L2A is a LSTM-based Seq2Seq model equipped with attention mechanism, which takes as input a linearized KG subgraph. It was included in [11] as a baseline. The results of L2A reported here are taken from [11]. We also include a Transformer-based encoder-decoder model [82] with copying mechanism that takes as input a linearized KG subgraph, i.e., a sequence of triples where each triple is represented as a sequence of tokens containing the subject name, predicate name and object name. Hence, after the transformation, a KG subgraph becomes a sequence of tokens. Note that the Transformer baseline included in our experiments encodes the word sequence that is linearized from a KG subgraph, while the MHQG+AE model encodes the triple set contained in a KG subgraph by removing the positional encoding in a regular Transformer architecture. Unlike MHQG+AE that takes as input a set of triple embeddings that are pretrained by a knowledge-base representation learning framework called TransE [61], the Transformer baseline takes a sequence of word embeddings as input. We used the open-source implementation [82] of the Transformer-based encoder-decoder model that is equipped with copying mechanism.

### B. Data and Metrics

Following [11], we used WebQuestions (WQ) and PathQuestions (PQ)<sup>1</sup> as our benchmarks where both of them use Freebase [83] as the underlying KG. The WQ dataset combines examples from WebQuestionsSP [84] and ComplexWebQuestions [85] where both of them are KBQA benchmarks that contain natural language questions, corresponding SPARQL

<sup>1</sup><https://github.com/liyuanfang/mhqg>

TABLE I: Data statistics. The min/max/avg statistics are reported on the queries and KG subgraph triples.

Data	# examples	# entities	# predicates	# triples	query length
WQ	22,989	25,703	672	2/99/5.8	5/36/15
PQ	9,731	7,250	378	2/3/2.7	8/25/14

TABLE II: Automatic evaluation results on WQ and PQ.

Method	WQ			PQ		
	BLEU-4	METEOR	ROUGE-L	BLEU-4	METEOR	ROUGE-L
L2A	6.01	25.24	26.95	17.00	19.72	50.38
Transformer	8.94	13.79	32.63	56.43	43.45	73.64
MHQG+AE	11.57	29.69	35.53	25.99	33.16	58.94
G2S+AE	<b>29.45</b>	30.96	<b>55.45</b>	<b>61.48</b>	44.57	<b>77.72</b>
G2S <sub>edge</sub> +AE	29.40	<b>31.12</b>	55.23	59.59	<b>44.70</b>	75.20

TABLE III: Human evaluation results ( $\pm$  standard deviation) on the WQ test set. The rating scale is from 1 to 5 (higher scores indicate better results).

Method	Syntactic	Semantic	Relevant	Overall
Transformer	<b>4.53 (0.18)</b>	<b>4.58 (0.22)</b>	2.65 (0.57)	3.92 (0.24)
G2S+AE	4.18 (0.30)	4.30 (0.27)	4.26 (0.34)	4.25 (0.26)
Ground-truth	4.30 (0.15)	4.50 (0.18)	<b>4.32 (0.32)</b>	<b>4.38 (0.19)</b>

TABLE IV: Ablation study on WQ and PQ.

Method	WQ			PQ		
	BLEU-4	METEOR	ROUGE-L	BLEU-4	METEOR	ROUGE-L
G2S+AE	<b>29.45</b>	<b>30.96</b>	<b>55.45</b>	<b>61.48</b>	<b>44.57</b>	<b>77.72</b>
G2S	28.43	30.13	54.44	60.68	44.07	75.94
G2S w/o copy	22.95	26.99	51.05	57.10	42.66	74.29

queries and answer entities. For each instance in WQ, in order to construct the KG subgraph, [11] converted its SPARQL query to return a subgraph instead of the answer entity, by changing it from a SELECT query to a CONSTRUCT query. The WQ dataset [11] contains 18,989/2,000/2,000 (train/development/test) examples. The PQ dataset [86] is similar to WQ except that the KG subgraph in PQ is a path between two entities that span two or three hops. The PQ dataset contains 9,793/1,000/1,000 (train/development/test) examples. Brief statistics of the two datasets are provided in Table I.

Following previous works, we use BLEU-4 [87], METEOR [88] and ROUGE-L [89] as automatic evaluation metrics. Initially, BLEU-4 and METEOR were designed for evaluating machine translation systems and ROUGE-L was designed for evaluating text summarization systems. We also conduct a human evaluation study on WQ. Generated questions are rated (i.e., range 1-5) based on whether they are syntactically correct, semantically correct and relevant to the KG subgraph. More specially, we conducted a small-scale (i.e., 50 random examples per system) human evaluation study on the WQ test set. We asked 6 human evaluators to give feedback on the quality of questions generated by a set of anonymized competing

systems. In each example, given a KG subgraph, target answers and an anonymized system output, they were asked to rate the quality of the output by answering the following three questions: i) is this generated question syntactically correct? ii) is this generated question semantically correct? and iii) is this generated question relevant to the KG subgraph and target answers? For each evaluation question, the rating scale is from 1 to 5 where a higher score means better quality (i.e., 1: Poor, 2: Marginal, 3: Acceptable, 4: Good, 5: Excellent). Responses from all evaluators were collected and averaged.

### C. Model Settings

We keep and fix the 300-dim GloVe [62] vectors for those words that occur more than twice in the training set. The dimensions of answer markup embeddings are set to 32 and 24 for WQ and PQ, respectively. We set the hidden state size of BiLSTM to 150 so that the concatenated state size for both directions is 300. The size of all other hidden layers is set to 300. We apply a variational dropout [90] rate of 0.4 after word embedding layers and 0.3 after RNN layers. The label smoothing ratio is set to 0.2. The number of GNN hops is set to 4. During training, in each epoch, we set the initial

teacher forcing probability to 0.8 and exponentially increase it to  $0.8 * 0.9999^i$  where  $i$  is the training step. In addition, partial teacher forcing is adopted, which means that when generating a sequence, some steps can be teacher forced and some not. We use Adam [91] as the optimizer. The learning rate is set to 0.001. We reduce the learning rate by a factor of 0.5 if the validation BLEU-4 score stops improving for three epochs. We stop the training when no improvement is seen for 10 epochs. We clip the gradient at length 10. The batch size is set to 30. The beam search width is set to 5. In the RL fine-tuning experiments, we set  $\gamma$  in the mixed loss function Eq. (8) to 0.02 for WQ and 0.07 for PQ. And the ratios of BLEU-4 score and ROUGE-L score for computing the reward are set to 1 and 0.02, respectively. We set the learning rate to 0.00001 and 0.00002 for WQ and PQ, respectively. All hyperparameters are tuned on the development set. Experiments were conducted on a machine which has an Intel i7-2700K CPU and an Nvidia Titan Xp GPU with 16GB RAM.

#### D. Experimental Results

Table II shows the evaluation results comparing our proposed models against other state-of-the-art baseline methods on WQ and PQ test sets. As we can see, our models outperform all baseline methods by a large margin on both benchmarks. This verifies the effectiveness of the proposed model. Besides, we can clearly see the advantages of GNN-based encoders for modeling KG subgraphs, by comparing our model with RNN-based (i.e., L2A) and Transformer-based (i.e., Transformer, MHGG+AE) baselines. Compared to our Graph2Seq model, both RNN-based and Transformer-based baselines ignore the explicit graph structure of a KG subgraph, which leads to degraded performance. Although RNNs are suitable for processing sequential data such as text, they are incapable of modeling graph-structured data such as a KG subgraph. To apply the RNN-based L2A model to a KG subgraph, [11] linearized the graph to a sequence during preprocessing. However, this inevitably ignores the rich structure information in the graph. Recently, the Transformer [16] has become a good alternative to the RNN when processing sequential data. Even though a Transformer [16] might be able to learn the semantic relations among the sequence elements through all-to-all attention, the explicit graph structure of a KG subgraph is totally discarded by the model. Given these limitations, as shown in our experiments, both of the two Transformer-based Seq2Seq baselines significantly underperform our GNN-based Graph2Seq model. Interestingly, the Transformer baseline performs reasonably well on PQ, but dramatically fails on WQ. We speculate this is because PQ is more friendly to sequential models such as Transformer as the KG subgraph in PQ is more like path-structure while the one in WQ is more like tree-structure.

We also compare two variants of our model (i.e., G2S vs. G2S<sub>edge</sub>) for handling multi-relational graphs. As shown in Table II, directly applying the BiGGNN encoder to a Levi graph which is converted from a KG subgraph works quite well. The proposed BiGGNN<sub>edge</sub> model can directly handle multi-relational graphs without modifying the input graph. However,

it performs slightly worse than the Levi graph solution. We can improve the modeling power of BiGGNN<sub>edge</sub> by updating edge embeddings in the message passing process and attending to edges in the attention mechanism. Currently, these two features are missing in BiGGNN<sub>edge</sub>. We leave these extensions as future work.

**Human evaluation and error analysis.** We conduct a human evaluation study to assess the quality of the questions generated by our model, the Transformer baseline, and the ground-truth data in terms of syntax, semantics and relevance metrics. In addition, an overall score is computed for each example by taking the average of the three scores. As shown in Table III, overall, we can see that our model achieves good results even compared to the ground-truth, and outperforms the Transformer baseline. Interestingly, we observe that the Transformer baseline gets high syntactic and semantic scores, but very poor relevant scores. After manually examining some generated questions, we noticed that it generates many fluent and meaningful questions that are by no means relevant to the given KG subgraph. However, our model is able to generate more relevant questions possibly by better capturing the KG semantics and the answer information. Our error analysis shows that main errors of our model occur in repeated words and grammatical errors in generated questions.

#### E. Ablation Study

As shown in Table IV, we perform an ablation study to assess the performance impacts of different model components. First of all, the node-level copying mechanism contributes a lot to the overall model performance. By turning it off, we observe significant performance drops on both benchmarks. This verifies our assumption that when generating questions from a KG subgraph, one usually directly copies named entities from the input KG subgraph to the output question. Besides, the answer information is also important for generating relevant questions. Even with the simple answer markup technique, we can see the performance boost on both benchmarks.

#### F. Model Analysis

1) *Effect of Node/Edge Embedding Initialization:* We empirically compare two different ways of initializing node/edge embeddings when applying the Graph2Seq model. As shown in Table V, encoding nodes and edges based on word embeddings of their textual attributes works better than based on their KG embeddings. This might be because it is difficult for a NN-based model to learn the gap between KG embeddings on the encoder side and word embeddings on the decoder side. With the word embedding-based encoding strategy, it is relatively easier for a model to learn the mapping from the input KG subgraph to the output NL question. It also seems that modeling local dependency within the subgraph without utilizing the global KG information is enough for generating meaningful questions from a KG subgraph.

2) *Impact of Directionality on GNN Encoder:* As shown in Table VI, we compare the performance of bidirectional Graph2Seq with unidirectional (i.e., forward and backward) Graph2Seq. We observe that performing only unidirectional

TABLE V: Effect of node/edge init. embeddings on WQ.

Method	BLEU-4	METEOR	ROUGE-L
w/ word emb.	28.43	30.13	54.44
w/ KG emb.	22.80	25.85	48.93

TABLE VI: Impact of directionality for G2S+AE on PQ.

Method	BLEU-4	METEOR	ROUGE-L
Bidirectional	61.48	44.57	77.72
Forward	59.59	42.72	75.82
Backward	59.12	42.66	75.03

TABLE VII: Results of RL-based G2S+AE on WQ.

Method	BLEU-4	METEOR	ROUGE-L
G2S+AE	29.45	30.96	55.45
G2S+AE+RL	29.80	31.29	55.51

TABLE VIII: Results of RL-based G2S+AE on PQ.

Method	BLEU-4	METEOR	ROUGE-L
G2S+AE	61.48	44.57	77.72
G2S+AE+RL	59.21	44.47	77.35

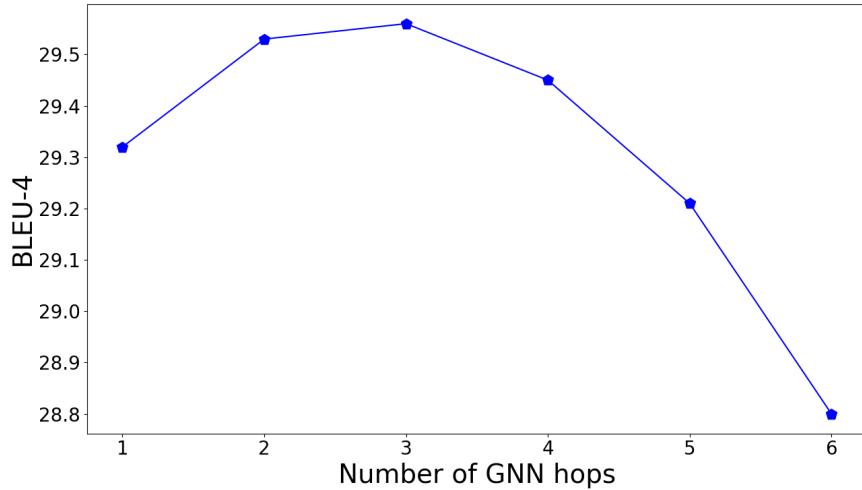


Fig. 2: Effect of the number of GNN hops for G2S+AE on PQ.

message passing when processing the KG subgraph degrades the performance.

3) *Results on Training the Model with a Hybrid Objective:* Table VII and Table VIII show the results of training our proposed G2S+AE model with a hybrid objective combining both cross-entropy loss and RL loss. We denote this variant as G2S+AE+RL. While the RL-based training strategy boosts the model performance on WQ, it does not help the model training on PQ.

4) *Effect of the Number of GNN Hops:* Fig. 2 shows the impact of the number of GNN hops when applying a GNN-

based encoder to encode the KG subgraph in WQ. It indicates that increasing the number of GNN hops can boost the model performance until some optimal value.

#### G. Case Study

As shown in Table IX, we conduct a case study to examine the quality of generated questions using different ablated systems. First of all, by initializing node/edge embeddings with KG embeddings, the model fails to generate reasonable questions. Besides, with the node-level copying mechanism, the model is able to directly copy the entity name “giza

TABLE IX: Generated questions on WQ test set. Target answers are underlined. For the sake of brevity, we only display the lowest level of the predicate hierarchy.

<b>KG subgraph:</b> ( <u>Egypt</u> , administrative_divisions, Cairo), ( <u>Giza Necropolis</u> , containedby, <u>Egypt</u> )
<b>Gold:</b> what country has the city of cairo and is home of giza necropolis ?
<b>G2S w/ KG emb.:</b> what country that contains cairo has cairo as its province ?
<b>G2S w/o copy:</b> where is the giza giza located in that has cairo ?
<b>G2S:</b> where is the giza necropolis located in that contains cairo ?
<b>G2S+AE:</b> what country that contains cairo is the location of giza necropolis ?

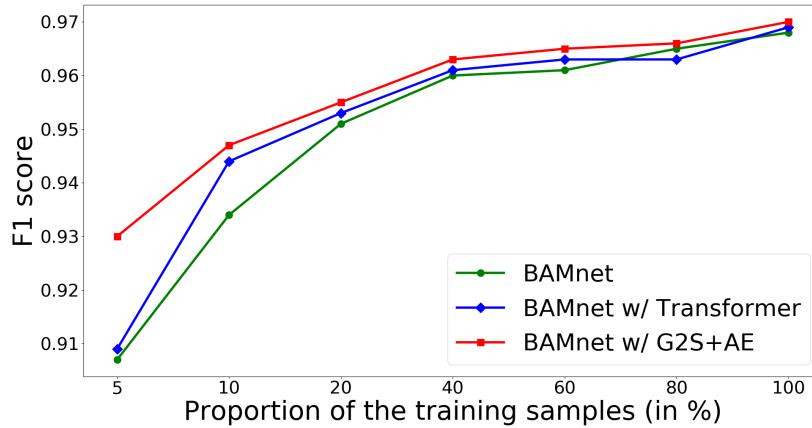


Fig. 3: Performance of QG-driven KBQA baseline under different proportions of training data.

necropolis” into the output question. Last, incorporating the answer information helps generate more relevant and specific questions.

#### H. QG-Driven Data Augmentation for QA

One of the most important applications of QG is to generate more training data for QA tasks. In this section, we use our proposed QG model to generate more questions for training KBQA methods. We use WQ as our KBQA benchmark, and randomly split it to 40%/20%/40% (train/dev/test) examples. As for the KBQA baseline, we use the state-of-the-art KBQA model called BAMnet [60] which directly retrieves answers from a KG by mapping questions and candidate answers into a joint embedding space. In order to examine the effect of QG-driven data augmentation on the KBQA task, we compare the BAMnet baseline with its two data augmentation variants, namely, BAMnet w/ Transformer and BAMnet w/ G2S+AE. More specifically, the BAMnet baseline is trained only on the part (i.e.,  $x\%$  of the whole training data) where gold questions are available, while the other two variants are trained on the combination of the gold questions and the questions automatically generated by two QG models. Note that given  $x\%$  training data, we randomly split it to 80%/20% (train/dev) for training a QG model.

We gradually increase the proportion (i.e.,  $x\%$ ) of the training data used for training KBQA models, and report the F1 score performance of the above three KBQA model variants. Here F1 score measures the overlap between the predicted and ground-truth answer set. Fig. 3 shows the results on improving the BAMnet baseline with automatically generated questions. Interestingly, both QG models consistently help improve the KBQA performance when varying  $x\%$  training data, and the performance boost is the most significant when training data is scarce. Notably, our G2S+AE model consistently outperforms the Transformer model in improving the KBQA performance.

## V. CONCLUSION

In this paper, we introduced a novel bidirectional Graph2Seq model for the KG-QG task. A novel node-level copying mechanism was proposed to allow directly copying node attributes from the KG subgraph to the output question. We explored different ways of initializing node/edge embeddings and handling multi-relational graphs. Our model outperforms existing methods by a significant margin on both WQ and PQ benchmarks. Future directions include exploring effective ways of initializing node/edge embeddings and utilizing answer information.

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