Advancing Abductive Reasoning in Knowledge Graphs through Complex Logical Hypothesis Generation

Anonymous ACL submission

Abstract

Abductive reasoning is the process of making educated guesses to provide explanations for observations. Although many applications require the use of knowledge for explanations, the utilization of abductive reasoning in conjunction with structured knowledge, such as a knowledge graph, remains largely unexplored. To fill this gap, this paper introduces the task of complex logical hypothesis generation, as an initial step towards abductive logical reasoning with KG. In this task, we aim to generate a complex logical hypothesis so that it can explain a set of observations. We find that the supervised trained generative model can generate logical hypotheses that are structurally closer to the reference hypothesis. However, when generalized to unseen observations, this training objective does not guarantee better hypothesis generation. To address this, we introduce the Reinforcement Learning from Knowledge Graph (RLF-KG) method, which minimizes differences between observations and conclusions drawn from generated hypotheses according to the KG. Experiments show that, with RLF-KG's assistance, the generated hypotheses provide better explanations, and achieve state-of-the-art results on three widely used KGs.

1 Introduction

Abductive reasoning plays a vital role in generating explanatory hypotheses for observed phenomena across various research domains (Haig, 2012). It is a powerful tool with wide-ranging applications. For example, in cognitive neuroscience, reverse inference (Calzavarini and Cevolani, 2022), which is a form of abductive reasoning, is crucial for inferring the underlying cognitive processes based on observed brain activation patterns. Similarly, in clinical diagnostics, abductive reasoning is recognized as a key approach for studying cause-and-effect relationships (Martini, 2023). Moreover, abductive reasoning is fundamental to the process of hypothesis generation in humans, animals, and computational machines (Magnani, 2023). Its significance extends beyond these specific applications and encompasses diverse fields of study. In this paper, we are focused on abductive reasoning with structured knowledge, specifically, a knowledge graph.

A typical knowledge graph (KG) stores information about entities, like people, places, items, and their relations in graph structures. Meanwhile, KG reasoning is the process that leverages knowledge graphs to infer or derive new information (Zhang et al., 2021a, 2022; Ji et al., 2022). In recent years, various logical reasoning tasks are proposed over knowledge graph, for example, answering complex queries expressed in logical structure (Hamilton et al., 2018; Ren and Leskovec, 2020), or conducting logical rule mining (Galárraga et al., 2015; Ho et al., 2018; Meilicke et al., 2019).

However, the abductive perspective of KG reasoning is crucial yet unexplored. Take the first example in Figure 1, where observation O_1 depicts five celebrities a user is following on a social media platform. The social network service provider is interested in using structured knowledge to explain the users' observed behavior. By leveraging a knowledge graph like Freebase (Bollacker et al., 2008), which includes some basic information about these people, a complex logical hypothesis H_1 can be derived. In this case, the knowledge graph suggests that they are all actors and screenwriters born in Los Angeles, expressed as H_1. Consider the second example in Figure 1, involving the interactions of a user on an e-commerce platform (O_2). Here, a structured hypothesis H_2 can explain the user's interest in $Apple$ products released in 2010 excluding $phones$. The third example, focused on medical diagnostics, features three diseases (O_3). The corresponding hypothesis H_3 indicates they are diseases $V_?$ with symptom V_1, and V_1 can be relieved by $Panadol$. From a general perspective, this problem illustrates the process of abductive logical reasoning with knowledge

Observations (O)	Hypotheses (H)	Interpretations
O_1 = {Grant Heslov, Jason Segel, Robert Towne, Ronald Bass, Rashida Jones}	$H_1 = V_? : Occupation(V_?, Actor) \wedge Occupation(V_?, ScreeeWriter) \wedge BornIn(V_?, LosAngeles)$	The actors and screenwriters born in Los Angeles
O_2 = {Ipad 1st Gen, Ipod touch 4th Gen, Apple TV 1st Gen}	$H_2 = V_? : Brand(V_?, Apple) \wedge ReleaseYear(V_?, 2010) \wedge \neg Type(V_?, Phone)$	The Apple products released in 2010 that are not phones
O_3 = {Covid-19, Seasonal Flu, Dysmenorrhea}	$H_3 = V_? , \exists V_1 : HaveSymptom(V_?, V_1) \wedge RelievedBy(V_1, Panadol)$	The disease whose symptoms can be relieved by Panadol

Figure 1: This figure shows some examples of observations and inferred logical hypotheses, expressed with discrepancies in interpretations.

graphs, seeking hypotheses that best explain given observation sets (Josephson and Josephson, 1996; Thagard and Shelley, 1997).

A straightforward approach to tackle this reasoning task is to employ a search-based method to explore potential hypotheses based on the given observation. However, this approach faces two significant challenges. The first challenge arises from the incompleteness of knowledge graphs (KGs), as searching-based methods heavily rely on the availability of complete information. In practice, missing edges in KGs can negatively impact the performance of search-based methods (Ren and Leskovec, 2020). The second challenge stems from the complexity of logically structured hypotheses. The search space for search-based methods becomes exponentially large when dealing with combinatorial numbers of candidate hypotheses. Consequently, the search-based method struggles to effectively and efficiently handle observations that require complex hypotheses for explanation.

To address these challenges, we propose a solution that leverages generative models within a supervised learning framework to generate logical hypotheses for a given set of observations. Our approach involves sampling hypothesis-observation pairs from observed knowledge graphs (Ren et al., 2020; Bai et al., 2023) and training a transformer-based generative model (Vaswani et al., 2017) using the teacher-forcing method. However, a potential limitation of supervised training is that it primarily focuses on capturing structural similarities, without necessarily guaranteeing improved explanations when applied to unseen observations. To overcome this limitation, we propose a method called reinforcement learning from the knowledge graph (RLF-KG). RLF-KG utilizes proximal policy optimization (PPO) (Schulman et al., 2017) to minimize the discrepancy between the observed evidence and the conclusion derived from the generated hypothesis. By incorporating reinforcement learning techniques, our approach aims to directly improve the explanatory capability of the generated hypotheses and ensure their effectiveness when generalized to unseen observations.

We evaluate the proposed methods for effectiveness and efficiency on three knowledge graphs: FB15k-237 (Toutanova and Chen, 2015), WN18RR (Toutanova and Chen, 2015), and DBpedia50 (Shi and Weninger, 2018). The results consistently demonstrate the superiority of our approach over supervised generation baselines and search-based methods, as measured by two evaluation metrics across all three datasets. Our contributions can be summarized as follows:

- We introduce the task of complex logical hypothesis generation, which aims to identify logical hypotheses that best explain a given set of observations. This task can be seen as a form of abductive reasoning with KGs.
- To address the challenges posed by the incompleteness of knowledge graphs and the complexity of logical hypotheses, we propose a generation-based method. This approach effectively handles these difficulties and enhances the quality of generated hypotheses.
- Additionally, we propose the Reinforcement Learning from Knowledge Graph (RLF-KG) technique. By incorporating feedback from the knowledge graph, RLF-KG further improves the hypothesis generation model. It minimizes the discrepancies between the observations and the conclusions derived from the generated hypotheses, leading to more accurate and reliable results.

2 Problem Formulation

In this task, a knowledge graph is denoted as $\mathcal{G} = (\mathcal{V}, \mathcal{R})$, where $\mathcal{V}$ is the set of vertices and $\mathcal{R}$ is the set of relation types. A *relation type* $r :\in \mathcal{R}$

maps vertex pairs to Boolean values, indicating the presence of an edge of type r. Namely, $r : \mathcal{V}\times\mathcal{V} \rightarrow \{\texttt{true}, \texttt{false}\}$ is defined by $r(u, v) = \texttt{true}$ if the directed edge (u, r, v) from u to v of type r exists in the KG and `false` otherwise.

We adopt the open-world assumption of KG (Drummond and Shearer, 2006), treating missing edges as unknown rather than false. The reasoning model can only access the observed KG $\mathcal{G}$, and evaluation is based on a hidden KG $\bar{\mathcal{G}}$, which encompasses the observed graph $\mathcal{G}$.

Abductive reasoning is a type of logical reasoning that involves making educated guesses to infer the most likely reasons for the observations (Josephson and Josephson, 1996; Thagard and Shelley, 1997). See Appendix A for clarification on abductive, deductive, and inductive reasoning. In this work, we focus on a specific abductive reasoning type in the context of knowledge graphs, formulated informally as Given a set of observations O and the knowledge graph $\mathcal{G}$, infer the hypothesis H that explains or describes O best. The detailed and precise definition is given below.

An *observation set* is a set of entities $O \subset \mathcal{V}$. A logical *hypothesis* H on a graph $\mathcal{G} = (\mathcal{V}, \mathcal{R})$ is defined as a predicate of a variable vertex $V_?$ in first-order logical form, including existential quantifiers, AND ($\wedge$), OR ($\vee$), and NOT ($\neg$). The hypothesis can always be written in disjunctive normal form,

$$H|_{\mathcal{G}}(V_?) = \exists V_1, \ldots, V_k : e_1 \vee \cdots \vee e_n, \quad (1)$$

$$e_i = r_{i1} \wedge \cdots \wedge r_{im_i}, \quad (2)$$

where each r_{ij} can take the forms: $r_{ij} = r(v, V)$, $r_{ij} = \neg r(v, V)$, $r_{ij} = r(V, V')$, $a_{ij} = \neg r(V, V')$, where v represents a fixed vertex, the V, V' represent variable vertices in $\{V_?, V_1, V_2, \ldots, V_k\}$, r is a relation type.

The subscript $|_{\mathcal{G}}$ denotes that the hypothesis is formulated based on the given graph $\mathcal{G}$. This means that all entities and relations in the hypothesis must exist in $\mathcal{G}$, and the domain for variable vertices is the entity set of $\mathcal{G}$. For example, please refer to Appendix B. The same hypothesis H can be applied to a different knowledge graph, $\mathcal{G}'$, provided that $\mathcal{G}'$ includes the entities and edges present in H. When the context is clear or the hypothesis pertains to a general statement applicable to multiple knowledge graphs (e.g., observed and hidden graphs), the symbol H is used without the subscript.

The *conclusion* of the hypothesis H on a graph $\mathcal{G}$, denoted by $[\![H]\!]_{\mathcal{G}}$, is the set of entities for which H holds true on $\mathcal{G}$:

$$[\![H]\!]_{\mathcal{G}} = \{V_? \in \mathcal{G} | H|_{\mathcal{G}}(V_?) = \texttt{true}\}. \quad (3)$$

Then, the formal definition of abductive reasoning in KG is as follows: Given an observation set $O = \{v_1, v_2, ..., v_k\}$ and the observed graph $\mathcal{G}$, abductive reasoning aims to find the hypothesis H on $\mathcal{G}$ whose conclusion on the hidden graph $\bar{\mathcal{G}}$, $[\![H]\!]_{\bar{\mathcal{G}}}$, is most similar to O. Similarity is measured using the Jaccard index:

$$\texttt{Jaccard}([\![H]\!]_{\bar{\mathcal{G}}}, O) = \frac{|[\![H]\!]_{\bar{\mathcal{G}}} \cap O|}{|[\![H]\!]_{\bar{\mathcal{G}}} \cup O|}. \quad (4)$$

In other words, the goal is to find a hypothesis H that maximizes $\texttt{Jaccard}([\![H]\!]_{\bar{\mathcal{G}}}, O)$.

3 Hypothesis Generation with RLF-KG

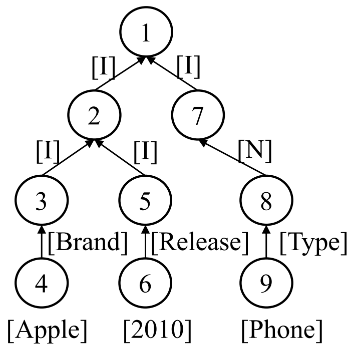
Our approach for abductive logical knowledge graph reasoning involves three steps: (1) Randomly sample observation-hypothesis pairs from the knowledge graph. (2) Train a generative model to generate hypotheses from observations using the sampled pairs. (3) Enhance the generative model using RLF-KG, leveraging reinforcement learning to minimize discrepancies between observations and generated hypotheses.

3.1 Supervised Training of Hypothesis Generation Model

In the first step, we randomly sample hypotheses from the observed training knowledge graph. To obtain the corresponding set of observations for each hypothesis, we conduct a graph search on the training graph, following the procedure described in the algorithms in Appendix D.

After sampling pairs of hypotheses and observations, we tokenize them in preparation for encoding and decoding by generative models. The entities in the observations are represented as unique tokens, such as `[Apple]` and `[Phone]`, as shown in Figure 2, and associated with token embedding vectors. To maintain consistency, we standardize the order of tokens for each observation, ensuring that permutations of the same observation set result in an identical sequence of unique tokens.

For hypothesis tokenization, we adopt a directed acyclic graph representation inspired by action-based parsing, as seen in other logical reasoning papers (Hamilton et al., 2018; Ren and Leskovec, 2020; Ren et al., 2020). Logical operations such as intersection, union, and negation are denoted



Hypothesis: $H = V_?\colon Brand(V_?, Apple) \wedge Release(V_?, 2010) \wedge \neg Type(V_?, Phone)$

$\Longleftrightarrow$

Nodes	Actions	Stack
1	[I]	1
2	[I]	1,2
3	[Brand]	1,2,3
4	[Apple]	1,2,3,4 $\rightarrow$ 1,2
5	[Release]	1,2,5
6	[2010]	1,2,5,6 $\rightarrow$ 1
7	[N]	1,7
8	[Type]	1,7,8
9	[Phone]	1,7,8,9 $\rightarrow$ empty

Tokens: [I][I][Brand][Apple][Release][2010][N][Type][Phone]

Figure 2: The figure demonstrates the tokenization process for hypotheses. We uniformly consider logical operations, relations, and entities as individual tokens, establishing a correspondence between the hypotheses and a sequence of tokens. For a more detailed explanation, please refer to the Appendix D.

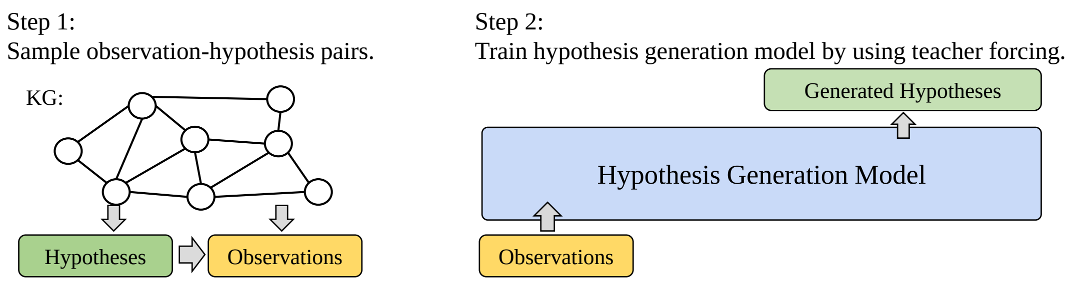


Figure 3: The first two steps of training a hypothesis generation model: In Step 1, we randomly sample logical hypotheses with diverse patterns and perform graph searches on the training graphs to obtain observations. These observations are then tokenized. In Step 2, a conditional generation model is trained to generate hypotheses based on given tokenized observations.

by special tokens `[I]`, `[U]`, and `[N]` respectively, following prior work (Bai et al., 2023). Relations and entities are also treated as unique tokens, for example, `[Brand]` and `[Apple]`. By utilizing a depth-first search algorithm (described in Appendix D), we generate a sequence of *actions* that represents the content and structure of the graph. This concludes the tokenization process for hypotheses. Conversely, Algorithm 3 is used to reconstruct a graph from an action sequence, serving as the detokenization process for logical hypotheses.

In the second step, we train a generative model on the sampled pairs. Let $\mathcal{O} = [o_1, o_2, ..., o_m]$ and $\mathcal{H} = [h_1, h_2, ..., h_n]$ denote the token sequences for observations and hypotheses respectively. The loss function for this example is defined as the standard sequence modeling loss:

$$\mathcal{L} = \log \rho(\mathcal{H}|\mathcal{O}) \tag{5}$$

$$= \log \sum_{i=1}^{n} \rho(h_i|\mathcal{O}, h_1, \ldots, h_{i-1}), \tag{6}$$

where ρ represents the generative model for conditional generation. We use a standard transformer model to implement this model. There are two approaches to utilizing the conditional generation model. The first approach follows the encoder-decoder architecture described in the original paper (Vaswani et al., 2017), where observation tokens are input to the transformer encoder, and shifted hypothesis tokens are input to the transformer decoder. The second approach involves concatenating observation and hypothesis tokens and using a decoder-only transformer for hypothesis generation. Both approaches can incorporate the RLF-KG.

3.2 Reinforcement Learning from Knowledge Graph Feedback (RLF-KG)

During the supervised training process, the model learns to generate hypotheses that have similar structures to reference hypotheses. However, higher structural similarity towards reference answers does not necessarily guarantee the ability to generate logical explanations, especially when encountering unseen observations during training.

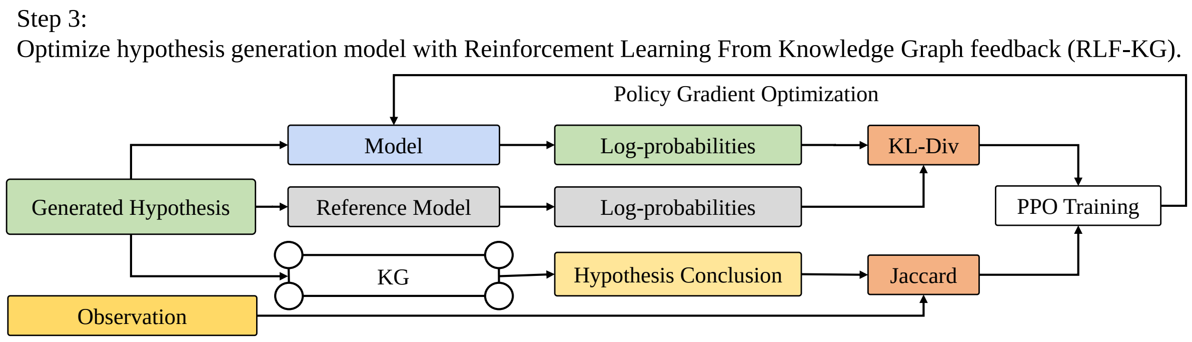


Figure 4: In Step 3, we employ RLF-KG to encourage the model to generate hypotheses that align more closely with the given observations from the knowledge graph. RLF-KG helps improve the consistency between the generated hypotheses and the observed evidence in the knowledge graph.

To address this limitation, we employ reinforcement learning (Ziegler et al., 2020) in conjunction with knowledge graph feedback (RLF-KG) to enhance the trained conditional generation model ρ. In Step 3, we initialize the model to be optimized, denoted as π, with the trained model ρ obtained from supervised training. We then treat ρ as the reference model. The token sequence representing the hypothesis, denoted as H, is de-tokenized to obtain the corresponding hypothesis H and its conclusion on the training graph $\mathcal{G}$, referred to as $[\![H]\!]_\mathcal{G}$.

As $\mathcal{G}$ represents the observed training graph, we utilize the Jaccard similarity between O and $[\![H]\!]_\mathcal{G}$ as a reliable and information leakage-free approximation for the objective of the abductive reasoning task, as defined in Equation 4.

To incorporate the feedback information from the training knowledge graph, we select this similarity measure as the reward function r. By using the Jaccard similarity as the reward function, we can effectively introduce the necessary feedback information to guide the RL process:

$$r(\mathcal{H}, \mathcal{O}) = \texttt{Jaccard}([\![H]\!]_\mathcal{G}, O) = \frac{|[\![H]\!]_\mathcal{G} \cap O|}{|[\![H]\!]_\mathcal{G} \cup O|}. \tag{7}$$

Building upon the approach outlined in (Ziegler et al., 2020), we enhance the reward function by incorporating a KL divergence penalty. This modification aims to discourage the optimized model π from generating hypotheses that deviate excessively from the reference model.

To train the model π, we employ the proximal policy optimization (PPO) algorithm (Schulman et al., 2017). The objective of the training process is to maximize the expected modified reward, which is calculated based on the training observation sets. By utilizing PPO and the modified reward function, we can effectively guide the model π towards generating hypotheses that strike a balance between similarity to the reference model and logical coherence. The formulas are as follows:

$$\mathbb{E}_{\mathcal{O}\sim D, \mathcal{H}\sim\pi(\cdot|\mathcal{O})}\left[r(\mathcal{H}, \mathcal{O}) - \beta \log \frac{\pi(\mathcal{H}|\mathcal{O})}{\rho(\mathcal{H}|\mathcal{O})}\right], \tag{8}$$

where D the is training observation distribution and $\pi(\cdot|\mathcal{O})$ is the conditional distribution of $\mathcal{H}$ on $\mathcal{O}$ modeled by the model π.

4 Experiment

We utilize three distinct knowledge graphs, namely FB15k-237 (Toutanova and Chen, 2015), DBpedia50 (Shi and Weninger, 2018), and WN18RR (Toutanova and Chen, 2015), for our experiments. Table 1 provides an overview of the number of training, evaluation, and testing edges, as well as the total number of nodes in each knowledge graph. To ensure consistency, we randomly partition the edges of these knowledge graphs into three sets - training, validation, and testing - using an 8:1:1 ratio. Consequently, we construct the training graph $\mathcal{G}_{\text{train}}$, validation graph $\mathcal{G}_{\text{valid}}$, and testing graph $\mathcal{G}_{\text{test}}$ by including the corresponding edges: training edges only, training + validation edges, and training + validation + testing edges, respectively.

Following the methodology outlined in Section 3.1, we proceed to sample pairs of observations and hypotheses. To ensure the quality and diversity of the samples, we impose certain constraints during the sampling process. Firstly, we restrict the size of the observation sets to a maximum of thirty-two elements. This limitation is enforced ensuring that the observations remain manageable. Additionally, specific constraints are applied to the validation and testing hypotheses. Each validation hypothesis must incorporate additional entities in the conclusion compared to the training graph,

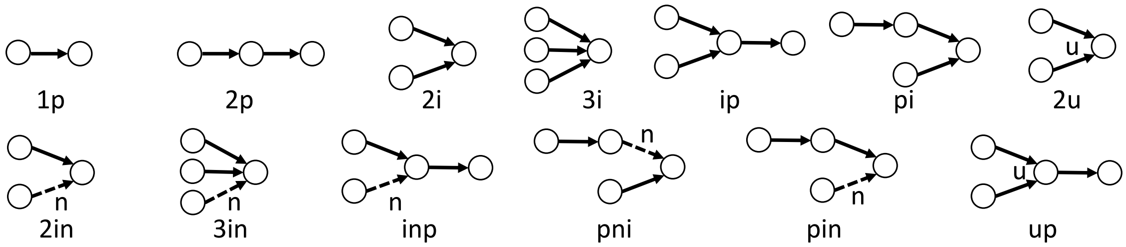


Figure 5: Our task involves considering thirteen distinct types of logical hypotheses. Each hypothesis type corresponds to a specific type of query graph, which is utilized during the sampling process. By associating each hypothesis type with a corresponding query graph, we ensure that a diverse range of hypotheses is sampled.

Dataset	Relations	Entities	Training	Validation	Testing	All Edges
FB15k-237	237	14,505	496,126	62,016	62,016	620,158
WN18RR	11	40,559	148,132	18,516	18,516	185,164
DBpedia50	351	24,624	55,074	6,884	6,884	68,842

Table 1: This figure provides basic information about the three knowledge graphs utilized in our experiments. The graphs are divided into standard sets of training, validation, and testing edges to facilitate the evaluation process.

while each testing hypothesis must have additional entities in the conclusion compared to the validation graph. This progressive increase in entity complexity ensures a challenging evaluation setting. The statistics of queries sampled for datasets are detailed in Appendix C.

In line with previous work on KG reasoning (Ren and Leskovec, 2020; Ren et al., 2020), we utilize thirteen pre-defined logical patterns to sample the hypotheses. Eight of these patterns, known as existential positive first-order (EPFO) hypotheses (1p/2p/2u/3i/ip/up/2i/pi), do not involve negations. The remaining five patterns are negation hypotheses (2in/3in/inp/pni/pin), which incorporate negations. It is important to note that the generated hypotheses may or may not match the type of the reference hypothesis. The structures of the hypotheses are visually presented in Figure 5, and the corresponding numbers of samples drawn for each hypothesis type can be found in Table 5.

4.1 Evaluation Metric

The quality of the generated hypothesis is primarily measured using the objective of abductive reasoning, as outlined in Section 2. Given an observation O and a generated hypothesis H, we employ a graph search algorithm to determine the conclusion of H on the evaluation graph $\mathcal{G}_{\text{test}}$, denoted as $[\![H]\!]_{\mathcal{G}_{\text{test}}}$. It is important to note that the evaluation graph contains ten percent of edges that were not observed during the training or validation stages.

The Jaccard metric $J_{\text{test}}(H, O)$ is then utilized to assess the quality of the generated hypothesis. This metric quantifies the similarity between the conclusion $[\![H]\!]_{\mathcal{G}_{\text{test}}}$ and the observation O. The Jaccard metric is given by:

$$\texttt{Jaccard}([\![H]\!]_{\mathcal{G}_{\text{test}}}, O) = \frac{|[\![H]\!]_{\mathcal{G}_{\text{test}}} \cap O|}{|[\![H]\!]_{\mathcal{G}_{\text{test}}} \cup O|}. \quad (9)$$

To further explore the similarity between the generated hypothesis and the reference hypothesis, we propose utilizing Smatch (Cai and Knight, 2013) to evaluate the structural resemblance of the hypothesis graphs. Originally designed for comparing semantic graphs, Smatch has been recognized as a suitable metric for evaluating complex logical queries, which can be treated as a specialized form of semantic graphs (Bai et al., 2023). The computation of the Smatch score on hypothesis graphs is described in detail in Appendix F. Denoted as $S(H, H_{\text{ref}})$, the Smatch score quantifies the similarity between the generated hypothesis H and the reference hypothesis H_{ref}.

4.2 Experiment Details

In this experiment, we use two transformer structures as the backbones of the generation model. For the encoder-decoder transformer structure, we use three encoder layers and three decoder layers. Each layer has eight attention heads with a hidden size of 512. Note that the positional encoding for the input observation sequence is disabled, as we believe that the order of the entities in the observation set does not matter. For the decoder-only structure, we use six layers, and the other hyperparameters are the same. In the supervised training process, we use AdamW optimizer and grid

Dataset	Model	1p	2p	2i	3i	ip	pi	2u	up	2in	3in	pni	pin	inp	Ave.
FB15k-237	Encoder-Decoder	0.626	0.617	0.551	0.513	0.576	0.493	0.818	0.613	0.532	0.451	0.499	0.529	0.533	0.565
	+ RLF-KG	**0.855**	**0.711**	**0.661**	**0.595**	**0.715**	**0.608**	**0.776**	**0.698**	**0.670**	**0.530**	**0.617**	**0.590**	**0.637**	**0.666**
	Decoder-Only	0.666	0.643	0.593	0.554	0.612	0.533	0.807	0.638	0.588	0.503	0.549	0.559	0.564	0.601
	+ RLF-KG	**0.789**	**0.681**	**0.656**	**0.605**	**0.683**	**0.600**	**0.817**	**0.672**	**0.672**	**0.560**	**0.627**	**0.596**	**0.626**	**0.660**
WN18RR	Encoder-Decoder	0.793	0.734	0.692	0.692	0.797	0.627	0.763	0.690	0.707	0.694	0.704	0.653	0.664	0.708
	+ RLF-KG	**0.850**	**0.778**	**0.765**	**0.763**	**0.854**	**0.685**	**0.767**	**0.719**	**0.743**	**0.732**	**0.738**	**0.682**	**0.710**	**0.753**
	Decoder-Only	0.760	0.734	0.680	0.684	0.770	0.614	0.725	0.650	0.683	0.672	0.688	0.660	0.677	0.692
	+ RLF-KG	**0.821**	**0.760**	**0.694**	**0.693**	**0.827**	**0.656**	**0.770**	**0.680**	**0.717**	**0.704**	**0.720**	**0.676**	**0.721**	**0.726**
DBpedia50	Encoder-Decoder	0.706	0.657	0.551	0.570	0.720	0.583	0.632	0.636	0.602	0.572	0.668	0.625	0.636	0.627
	+ RLF-KG	**0.842**	**0.768**	**0.636**	**0.639**	**0.860**	**0.667**	**0.714**	**0.758**	**0.699**	**0.661**	**0.775**	**0.716**	**0.769**	**0.731**
	Decoder-Only	0.739	0.692	0.426	0.434	0.771	0.527	**0.654**	0.688	0.602	0.563	0.663	**0.640**	0.701	0.623
	+ RLF-KG	**0.777**	**0.701**	**0.470**	**0.475**	**0.821**	**0.534**	0.646	**0.702**	**0.626**	**0.575**	**0.696**	0.626	**0.713**	**0.643**

Table 2: The detailed Jaccard performance of various methods.

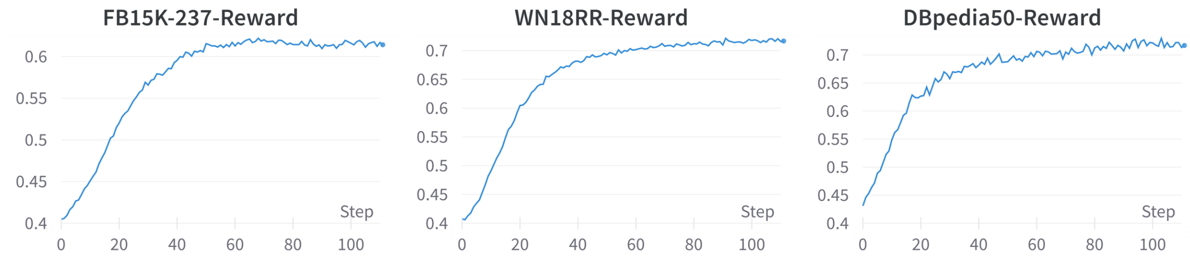


Figure 6: The curve of the reward values of RLF-KG training over three different datasets.

search to find hyper-parameters. For the encoder-decoder structure, the learning rate is 0.0001 with the resulting batch size of 768, 640, and 256 for FB15k-237, WN18RR, and DBpedia, respectively. For the decoder-only structure, the learning rate is 0.00001 with batch-size of 256, 160, and 160 for FB15k-237, WN18RR, and DBpedia respectively, and linear warming up of 100 steps. In the reinforcement learning process, we use the dynamic adjustment of the penalty coefficient β (Ouyang et al., 2022). More detailed hyperparameters are shown in Appendix H. All the experiments can be conducted on a single GPU with 24GB memory.

4.3 Experiment Results

We validate RLF-KG effectiveness by comparing the Jaccard metric of the model before and after this process. Table 2 displays performance across thirteen hypothesis types on FB15k-237, WN18RR, and DBpedia50. It illustrates Jaccard indices between observations and conclusions of generated hypotheses from the test graph. The encoder-decoder and the decoder-only transformers are assessed under fully supervised training on each dataset. Additionally, performance is reported when models collaborate with reinforcement learning from knowledge graph feedback (RLF-KG).

We notice RLF-KG consistently enhances hypothesis generation across three datasets, improving both encoder-decoder and decoder-only models. This can be explained by RLF-KG's ability to incorporate knowledge graph information into the generation model, diverging from simply generating hypotheses akin to reference hypotheses.

Additionally, after the RLF-KG training, the encoder-decoder model surpasses the decoder-only structured transformer model. This is due to the task's nature, where generating a sequence of tokens from an observation set does not necessitate the order of the observation set. Figure 6 supplements the previous statement by illustrating the increasing reward throughout the PPO process. We also refer readers to Appendix J for qualitative examples demonstrating the improvement in the generated hypotheses for the same observation.

4.4 Adding Structural Reward to PPO

In this part, we explore the potential benefits of incorporating structural similarity into the reward function used in PPO training. While RLF-KG originally relies on the Jaccard index, we consider adding the Smatch score, a measure of structural differences between generated and sampled hypotheses. As introduced before, the structural similarity can be measured by the Smatch score. We also conducted further experiments to also include $S(H, H_{\text{ref}})$ as an additional term of the reward function, and the results are shown in Table 3. As Smatch scores suggest, by incorporating the structural reward, the model can indeed generate

	FB15k-237		WN18RR		DBpedia50	
	Jaccard	Smatch	Jaccard	Smatch	Jaccard	Smatch
Encoder-Decoder	0.565	**0.602**	0.708	**0.558**	0.627	0.486
+ RLF-KG (Jaccard)	**0.666**	0.530	0.753	0.540	**0.731**	**0.541**
+ RLF-KG (Jaccard + Smatch)	0.660	0.568	**0.757**	0.545	0.696	0.532
Decoder-Only	0.601	**0.614**	0.692	**0.564**	0.623	**0.510**
+ RLF-KG (Jaccard)	**0.660**	0.598	**0.726**	0.518	0.643	0.492
+ RLF-KG (Jaccard + Smatch)	0.656	0.612	0.713	0.540	**0.645**	0.504

Table 3: The Jaccard and Smatch performance of different reward functions.

Method	FB15k-237			WN18RR			DBpedia50		
	Runtime	Jaccard	Smatch	Runtime	Jaccard	Smatch	Runtime	Jaccard	Smatch
Brute-force Search	16345 mins	0.635	0.305	4084 mins	0.742	0.322	1132 mins	0.702	0.322
Generation + RLF-KG	**264 mins**	**0.666**	**0.530**	**32 mins**	**0.753**	**0.540**	**5 mins**	**0.731**	**0.541**

Table 4: Performance on testing data and runtime for inference for various methods on testing data.

hypotheses that are closer to the reference hypotheses. However, the Jaccard scores show that with structural information incorporated, the overall performance is comparable to or slightly worse than the original reward function. The detailed Smatch scores by query types can be found in Appendix G

4.5 Comparison Between Search Methods

In this section, we compare inference time and performance between the generation-based and search-based methods. To do this comparison, we introduce a brute-force search algorithm. For each given observation, the algorithm, as detailed in Appendix I, explores all potential 1p hypotheses within the training graph and selects the one with the highest Jaccard similarity on the training graph. Table 4 shows that, notably, generation-based models of both architectures consistently exhibit significantly faster performance compared to the search-based method. Table 4 shows that, while our generation model only slightly overperforms the search-based method in Jaccard performance, it is significantly better in Smatch performance.

5 Related Work

The problem of abductive knowledge graph reasoning shares connections with various other knowledge graph reasoning tasks, including knowledge graph completion, complex logical query answering, and rule mining. Rule mining is a line of work focusing on inductive logical reasoning, namely discovering logical rules over the knowledge graph. Various methods are proposed in this line of work (Galárraga et al., 2015; Ho et al., 2018; Meilicke et al., 2019; Cheng et al., 2022, 2023).

Complex logical query answering is a task of answering logically structured queries on KG. Query embedding primary focus is the enhancement of embedding structures for encoding sets of answers (Hamilton et al., 2018; Sun et al., 2020; Liu et al., 2021). For instance, (Ren and Leskovec, 2020) and (Zhang et al., 2021b) introduce the utilization of geometric structures such as rectangles and cones within hyperspace to represent entities. Neural MLP (Mixer) (Amayuelas et al., 2022) use MLP and MLP-Mixer as the operators. (Bai et al., 2022) suggests employing multiple vectors to encode queries, thereby addressing the diversity of answer entities. FuzzQE (Chen et al., 2022) uses fuzzy logic to represent logical operators. Probabilistic distributions can also serve as a means of query encoding (Choudhary et al., 2021a,b), with examples including Beta Embedding (Ren and Leskovec, 2020) and Gamma Embedding (Yang et al., 2022).

6 Conclusion

In summary, this paper has introduced the task of abductive logical knowledge graph reasoning. Meanwhile, this paper has proposed a generation-based method to address knowledge graph incompleteness and reasoning efficiency by generating logical hypotheses. Furthermore, this paper demonstrates the effectiveness of our proposed reinforcement learning from knowledge graphs (RLF-KG) to enhance our hypothesis generation model by leveraging feedback from knowledge graphs.

Limitations

Our proposed methods and techniques in the paper are evaluated on a specific set of knowledge graphs, namely FB15k-237, WN18RR, and DBpedia50. It is unclear how well these approaches would perform on other KGs with different characteristics or domains. Meanwhile, knowledge graphs can be massive and continuously evolving, our method is not yet able to address the dynamic nature of knowledge evolutions, like conducting knowledge editing automatically. It is important to note that these limitations should not undermine the significance of the work but rather serve as areas for future research and improvement.

References

Alfonso Amayuelas, Shuai Zhang, Susie Xi Rao, and Ce Zhang. 2022. Neural methods for logical reasoning over knowledge graphs. In *The Tenth International Conference on Learning Representations, ICLR 2022, Virtual Event, April 25-29, 2022*. OpenReview.net.

Jiaxin Bai, Zihao Wang, Hongming Zhang, and Yangqiu Song. 2022. Query2Particles: Knowledge graph reasoning with particle embeddings. In *Findings of the Association for Computational Linguistics: NAACL 2022*, pages 2703–2714, Seattle, United States. Association for Computational Linguistics.

Jiaxin Bai, Tianshi Zheng, and Yangqiu Song. 2023. Sequential query encoding for complex query answering on knowledge graphs. *Transactions on Machine Learning Research*.

Kurt D. Bollacker, Colin Evans, Praveen K. Paritosh, Tim Sturge, and Jamie Taylor. 2008. Freebase: a collaboratively created graph database for structuring human knowledge. In *Proceedings of the ACM SIGMOD International Conference on Management of Data, SIGMOD 2008, Vancouver, BC, Canada, June 10-12, 2008*, pages 1247–1250. ACM.

Shu Cai and Kevin Knight. 2013. Smatch: an evaluation metric for semantic feature structures. In *Proceedings of the 51st Annual Meeting of the Association for Computational Linguistics, ACL 2013, 4-9 August 2013, Sofia, Bulgaria, Volume 2: Short Papers*, pages 748–752. The Association for Computer Linguistics.

Fabrizio Calzavarini and Gustavo Cevolani. 2022. Abductive reasoning in cognitive neuroscience: Weak and strong reverse inference. *Synthese*, 200(2):1–26.

Xuelu Chen, Ziniu Hu, and Yizhou Sun. 2022. Fuzzy logic based logical query answering on knowledge graphs. In *Thirty-Sixth AAAI Conference on Artificial Intelligence, AAAI 2022, Thirty-Fourth Conference on Innovative Applications of Artificial Intelligence, IAAI 2022, The Twelveth Symposium on Educational Advances in Artificial Intelligence, EAAI 2022 Virtual Event, February 22 - March 1, 2022*, pages 3939–3948. AAAI Press.

Kewei Cheng, Nesreen K. Ahmed, and Yizhou Sun. 2023. Neural compositional rule learning for knowledge graph reasoning. In *The Eleventh International Conference on Learning Representations, ICLR 2023, Kigali, Rwanda, May 1-5, 2023*. OpenReview.net.

Kewei Cheng, Jiahao Liu, Wei Wang, and Yizhou Sun. 2022. Rlogic: Recursive logical rule learning from knowledge graphs. In *KDD '22: The 28th ACM SIGKDD Conference on Knowledge Discovery and Data Mining, Washington, DC, USA, August 14 - 18, 2022*, pages 179–189. ACM.

Nurendra Choudhary, Nikhil Rao, Sumeet Katariya, Karthik Subbian, and Chandan K. Reddy. 2021a. Probabilistic entity representation model for reasoning over knowledge graphs. In *Advances in Neural Information Processing Systems 34: Annual Conference on Neural Information Processing Systems 2021, NeurIPS 2021, December 6-14, 2021, virtual*, pages 23440–23451.

Nurendra Choudhary, Nikhil Rao, Sumeet Katariya, Karthik Subbian, and Chandan K. Reddy. 2021b. Self-supervised hyperboloid representations from logical queries over knowledge graphs. In *WWW '21: The Web Conference 2021, Virtual Event / Ljubljana, Slovenia, April 19-23, 2021*, pages 1373–1384. ACM / IW3C2.

Igor Douven. 2021. Abduction. In Edward N. Zalta, editor, *The Stanford Encyclopedia of Philosophy*, Summer 2021 edition. Metaphysics Research Lab, Stanford University.

Nick Drummond and Rob Shearer. 2006. The open world assumption. In *eSI Workshop: The Closed World of Databases meets the Open World of the Semantic Web*, volume 15, page 1.

Luis Galárraga, Christina Teflioudi, Katja Hose, and Fabian M. Suchanek. 2015. Fast rule mining in ontological knowledge bases with AMIE+. *VLDB J.*, 24(6):707–730.

Brian D. Haig. 2012. *Abductive Learning*, pages 10–12. Springer US, Boston, MA.

William L. Hamilton, Payal Bajaj, Marinka Zitnik, Dan Jurafsky, and Jure Leskovec. 2018. Embedding logical queries on knowledge graphs. In *Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, December 3-8, 2018, Montréal, Canada*, pages 2030–2041.

Vinh Thinh Ho, Daria Stepanova, Mohamed H. Gad-Elrab, Evgeny Kharlamov, and Gerhard Weikum. 2018. Rule learning from knowledge graphs guided by embedding models. In *The Semantic Web - ISWC 2018 - 17th International Semantic Web Conference,* *Monterey, CA, USA, October 8-12, 2018, Proceedings, Part I*, volume 11136 of *Lecture Notes in Computer Science*, pages 72–90. Springer.

Shaoxiong Ji, Shirui Pan, Erik Cambria, Pekka Marttinen, and Philip S. Yu. 2022. A survey on knowledge graphs: Representation, acquisition, and applications. *IEEE Trans. Neural Networks Learn. Syst.*, 33(2):494–514.

John R Josephson and Susan G Josephson. 1996. *Abductive inference: Computation, philosophy, technology*. Cambridge University Press.

Lihui Liu, Boxin Du, Heng Ji, ChengXiang Zhai, and Hanghang Tong. 2021. Neural-answering logical queries on knowledge graphs. In *KDD '21: The 27th ACM SIGKDD Conference on Knowledge Discovery and Data Mining, Virtual Event, Singapore, August 14-18, 2021*, pages 1087–1097. ACM.

Lorenzo Magnani. 2023. *Handbook of Abductive Cognition*. Springer International Publishing.

Carlo Martini. 2023. *Abductive Reasoning in Clinical Diagnostics*, pages 467–479. Springer International Publishing, Cham.

Christian Meilicke, Melisachew Wudage Chekol, Daniel Ruffinelli, and Heiner Stuckenschmidt. 2019. Anytime bottom-up rule learning for knowledge graph completion. In *Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence, IJCAI 2019, Macao, China, August 10-16, 2019*, pages 3137–3143. ijcai.org.

Long Ouyang, Jeffrey Wu, Xu Jiang, Diogo Almeida, Carroll L. Wainwright, Pamela Mishkin, Chong Zhang, Sandhini Agarwal, Katarina Slama, Alex Ray, John Schulman, Jacob Hilton, Fraser Kelton, Luke Miller, Maddie Simens, Amanda Askell, Peter Welinder, Paul F. Christiano, Jan Leike, and Ryan Lowe. 2022. Training language models to follow instructions with human feedback. In *NeurIPS*.

Hongyu Ren, Weihua Hu, and Jure Leskovec. 2020. Query2box: Reasoning over knowledge graphs in vector space using box embeddings. In *8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020*. OpenReview.net.

Hongyu Ren and Jure Leskovec. 2020. Beta embeddings for multi-hop logical reasoning in knowledge graphs. In *Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual*.

John Schulman, Filip Wolski, Prafulla Dhariwal, Alec Radford, and Oleg Klimov. 2017. Proximal Policy Optimization Algorithms. ArXiv:1707.06347 [cs].

Baoxu Shi and Tim Weninger. 2018. Open-world knowledge graph completion. In *Proceedings of the Thirty-Second AAAI Conference on Artificial Intelligence, (AAAI-18), the 30th innovative Applications of Artificial Intelligence (IAAI-18), and the 8th AAAI Symposium on Educational Advances in Artificial Intelligence (EAAI-18), New Orleans, Louisiana, USA, February 2-7, 2018*, pages 1957–1964. AAAI Press.

Haitian Sun, Andrew O. Arnold, Tania Bedrax-Weiss, Fernando Pereira, and William W. Cohen. 2020. Faithful embeddings for knowledge base queries. In *Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual*.

Paul Thagard and Cameron Shelley. 1997. Abductive reasoning: Logic, visual thinking, and coherence. In *Logic and Scientific Methods: Volume One of the Tenth International Congress of Logic, Methodology and Philosophy of Science, Florence, August 1995*, pages 413–427. Springer.

Kristina Toutanova and Danqi Chen. 2015. Observed versus latent features for knowledge base and text inference. In *Proceedings of the 3rd Workshop on Continuous Vector Space Models and their Compositionality, CVSC 2015, Beijing, China, July 26-31, 2015*, pages 57–66. Association for Computational Linguistics.

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, and Illia Polosukhin. 2017. Attention is all you need. In *Advances in Neural Information Processing Systems 30: Annual Conference on Neural Information Processing Systems 2017, December 4-9, 2017, Long Beach, CA, USA*, pages 5998–6008.

Dong Yang, Peijun Qing, Yang Li, Haonan Lu, and Xiaodong Lin. 2022. Gammae: Gamma embeddings for logical queries on knowledge graphs. In *Proceedings of the 2022 Conference on Empirical Methods in Natural Language Processing, EMNLP 2022, Abu Dhabi, United Arab Emirates, December 7-11, 2022*, pages 745–760. Association for Computational Linguistics.

Jing Zhang, Bo Chen, Lingxi Zhang, Xirui Ke, and Haipeng Ding. 2021a. Neural, symbolic and neural-symbolic reasoning on knowledge graphs. *AI Open*, 2:14–35.

Wen Zhang, Jiaoyan Chen, Juan Li, Zezhong Xu, Jeff Z. Pan, and Huajun Chen. 2022. Knowledge graph reasoning with logics and embeddings: Survey and perspective. *CoRR*, abs/2202.07412.

Zhanqiu Zhang, Jie Wang, Jiajun Chen, Shuiwang Ji, and Feng Wu. 2021b. Cone: Cone embeddings for multi-hop reasoning over knowledge graphs. In *Advances in Neural Information Processing Systems 34: Annual Conference on Neural Information Processing Systems 2021, NeurIPS 2021, December 6-14, 2021, virtual*, pages 19172–19183.

Daniel M. Ziegler, Nisan Stiennon, Jeffrey Wu, Tom B. Brown, Alec Radford, Dario Amodei, Paul Christiano, and Geoffrey Irving. 2020. Fine-Tuning Language Models from Human Preferences. ArXiv:1909.08593 [cs, stat].

A Clarification on Abductive, Deductive, and Inductive Reasoning

Here we use simple syllogisms to explain the connections and differences between abductive reasoning and the other two types of reasoning, namely, deductive and inductive reasoning. In deductive reasoning, the inferred conclusion is necessarily true if the premises are true. Suppose we have a major premise P_1: *All men are mortal*, a minor premise P_2: *Socrates is a man*, then we can conclude C that *Socrates is mortal*. This can also be expressed as the inference $\frac{P_1 \wedge P_2}{C}$. On the other hand, abductive reasoning aims to explain an observation and is non-necessary, i.e., the inferred hypothesis is not guaranteed to be true. We also start with a premise P: *All cats like catching mice*, and then we have some observation O: *Katty like catching mice*. The abduction gives a simple yet most probable hypothesis H: *Katty is a cat*, as an explanation. This can also be written as the inference $\frac{P \wedge O}{H}$. Different than deductive reasoning, the observation O should be entailed by the premise P and the hypotheses H, which can be expressed by the implication $P \wedge H \implies O$. The other type of non-necessary reasoning is inductive reasoning, where, in contrast to the appeal to explanatory considerations in abductive reasoning, there is an appeal to observed frequencies (Douven, 2021). For instance, premises P_1: *Most Math students learn linear algebra in their first year* and P_2: Alice is a Math student infer H: *Alice learned linear algebra in her first year*, i.e., $\frac{P_1 \wedge P_2}{H}$. Note that the inference rules in the last two examples are not strictly logical implications.

It is worth mentioning that there might be different definitions or interpretations of these forms of reasoning.

B Example of Observation-Hypothesis Pair

For example, observation O can be a set of name entities like $\{GrantHeslov, JasonSegel, RobertTowne, RonaldBass, RashidaJones\}$. Given this observation, an abductive reasoner is required to give the logical hypothesis that best explains it. For the above example, the expected hypothesis H in natural language is that they are *actors* and *screenwriters*, and they are also born in *Los Angeles*. Mathematically, the hypothesis H can be represented by a logical expression of the facts of the KG: $H(V) = Occupation(V, Actor) \wedge Occupation(V, ScreenWriter) \wedge BornIn(V, LosAngeles)$. Although the logical expression here only contains logical conjunction AND ($\wedge$), we consider more general first-order logical form as defined in Section 2.

C Statistics of Queries Sampled for Datasets

Table 5 presents the numbers of queries sampled for each dataset in each stage.

D Algorithm for Sampling Observation-Hypothesis Pairs

Algorithm 1 is designed for sampling complex hypotheses from a given knowledge graph. Given a knowledge graph $\mathcal{G}$ and a hypothesis type T, the algorithm starts with a random node v and proceeds to recursively construct a hypothesis that has v as one of its conclusions and adheres the type T. During the recursion process, the algorithm examines the last operation in the current hypothesis. If the operation is a *projection*, the algorithm randomly selects one of v's in-edge (u, r, v). Then, the algorithm calls the recursion on node u and the sub-hypothesis type of T again. If the operation is an *intersection*, it applies recursion on the sub-hypotheses and the same node v. If the operation is a *union*, it applies recursion on one sub-hypothesis with node v and on other sub-hypotheses with an arbitrary node, as union only requires one of the sub-hypotheses to have v as an answer node. The recursion stops when the current node contains an entity.

E Algorithms for Conversion between Queries and Actions

We here present the details of tokenizing the hypothesis graph (Algorithm 2), and formulating a graph according to the tokens, namely the process of de-tokenization (Algorithm 3). Inspired by the action-based semantic parsing algorithms, we view tokens as actions. It is worth noting that we employ the symbols G, V, E for the hypothesis graph to differentiate it from the knowledge graph.

F Details of using Smatch to evaluate structural differneces of queries

Smatch (Cai and Knight, 2013) is an evaluation metric for Abstract Meaning Representation

Algorithm 1 Sampling Hypothesis According to Type

Input Knowledge graph $\mathcal{G}$, hypothesis type T
Output Hypothesis sample

function $\textsc{GroundType}(\mathcal{G}, T, t)$
  if $T.operation = p$ **then**
    $(h, r) \leftarrow \textsc{Sample}(\{(h, r) | (h, r, t) \in \mathcal{E}(\mathcal{G})\})$
    $\hat{T} \leftarrow$ the only subtype in $T.SubTypes$
    $H \leftarrow \textsc{GroundType}(\mathcal{G}, \hat{T}, h)$
    return (p, r, H)
  else if $T.operation = i$ **then**
    $SubHypotheses \leftarrow \emptyset$
    for $\hat{T} \in T.SubTypes$ **do**
      $H \leftarrow \textsc{GroundType}(\mathcal{G}, \hat{T}, t)$
      $SubHypotheses.\textsc{pushback}(H)$
    end for
    return $(i, SubHypotheses)$
  else if $T.operation = u$ **then**
    $SubHypotheses \leftarrow \emptyset$
    for $\hat{T} \in T.SubTypes$ **do**
      if $\hat{T}$ is the first subtype **then**
        $H \leftarrow \textsc{GroundType}(\mathcal{G}, \hat{T}, t)$
      else
        $\hat{t} \leftarrow \textsc{Sample}(\mathcal{V}(\mathcal{G}))$
        $H \leftarrow \textsc{GroundType}(\mathcal{G}, \hat{T}, \hat{t})$
      end if
      $SubHypotheses.\textsc{pushback}(H)$
    end for
    return $(u, SubHypotheses)$
  else if $T.operation = e$ **then**
    return (e, t)
  end if
end function
$v \leftarrow \textsc{Sample}(\mathcal{V}(\mathcal{G}))$
return $\textsc{GroundType}(\mathcal{G}, T, v)$

Dataset	Training Samples		Validation Samples		Testing Samples	
	Each Type	Total	Each Type	Total	Each Type	Total
FB15k-237	496,126	6,449,638	62,015	806,195	62,015	806,195
WN18RR	148,132	1,925,716	18,516	240,708	18,516	240,708
DBpedia50	55,028	715,364	6,878	89,414	6,878	89,414

Table 5: The detailed information about the queries used for training, validation, and testing.

Algorithm 2 HypothesisToActions

Input Hypothesis plan graph G
Output Action sequence A

function DFS(G, t, A)
  if t is an anchor node **then**
    $action \leftarrow$ entity associated with t
  else
    $action \leftarrow$ operator associated with the first in-edge of t
  end if
  $A.\textsc{PushBack}(action)$
  for all in-edges to t in G (h, r, t) **do**
    DFS(G, h, A)
  end for
end function
$root \leftarrow$ the root of G
$A \leftarrow$ DFS($G, root, \emptyset$)
return A

Algorithm 3 ActionsToHypothesis

Input Action sequence A
Output Hypothesis plan graph G

$S \leftarrow$ an empty stack
Create an map deg. $deg[i] = deg[u] = 2$ and $= 1$ otherwise.
$V \leftarrow \emptyset, E \leftarrow \emptyset$
for $a \in A$ **do**
  Create a new node h, $V \leftarrow V \cup \{h\}$
  if $S \neq \emptyset$ **then**
    $(t, operator, d) \leftarrow S.\textsc{Top}$
    $E \leftarrow E \cup \{(h, operator, t)\}$
  end if
  if a represents an anchor **then**
    Mark h as an anchor with entity a
    while $S \neq \emptyset$ **do**
      $(t, operator, d) \leftarrow S.\textsc{Pop}$
      $d \leftarrow d - 1$
      if $d > 0$ **then**
        $S.\textsc{PushBack}((t, operator, d))$
        Break
      end if
    end while
  else
    $S.\textsc{PushBack}((h, a, deg[a]))$
  end if
end for
$G \leftarrow (V, E)$
return G

(AMR) graphs. An AMR graph is a directed acyclic graph with two types of nodes: variable nodes and concept nodes, and three types of edges:

- Instance edges, which connect a variable node to a concept node and are labeled literally "instance". Every variable node must have exactly one instance edge, and vice versa.
- Attribute edges, which connect a variable node to a concept node and are labeled with attribute names.
- Relation edges, which connect a variable node to another variable node and are labeled with relation names.

Given a predicted AMR graph G_{p} and the gold AMR graph G_{g}, the Smatch score of G_{p} with respect to G_{g} is denoted by $\texttt{Smatch}(G_{\mathrm{p}}, G_{\mathrm{g}})$. $\texttt{Smatch}(G_{\mathrm{p}}, G_{\mathrm{g}})$ is obtained by finding an approximately optimal mapping between the variable nodes of the two graphs and then matching the edges of the graphs.

Our hypothesis graph is similar to the AMR graph, in:

- The nodes are both categorized as fixed nodes and variable nodes
- The edges can be categorized into two types: edges from a variable node to a fixed node and edges from a variable node to another variable node. And edges are labeled with names.

However, they are different in that the AMR graph requires every variable node to have instance edges, while the hypothesis graph does not.

The workaround for leveraging the Smatch score to measure the similarity between hypothesis graphs is creating an instance edge from every entity to some virtual node. Formally, given a hypothesis H with hypothesis graph $G(H)$, we create a new hypothesis graph $G_A(H)$ to accommodate the AMR settings as follows: First, we initialize $G_A(H) = G(H)$. Then, create a new relation type $instance$ and add a virtual node v' into $G_A(H)$. Finally, for every variable node $v \in G(H)$, we add a relation $instance(v, v')$ into $G_A(H)$. Then, given a predicted hypothesis H_p and a gold hypothesis H_g, the Smatch score is defined as

$$S(H_p, H_g) = \texttt{Smatch}(G_A(H_p), G_A(H_g)). \quad (10)$$

Through this conversion, a variable entity v_g of H_g is mapped to a variable entity v_p of H_p if and only if $instance(v_g, v')$ is matched with $instance(v_p, v')$. This modification does not affect the overall algorithm for finding the optimal mapping between variable nodes and hence gives a valid and consistent similarity score. However, this adds an extra point for matching between instance edges, no matter how the variable nodes are mapped.

G Detailed Smatch Scores by Query Types

Tables 6 and 7 show the detailed Smatch performance of various methods.

H Hyperparameters of the RL Process

The PPO hyperparameters are shown in Table 8. We warm-uped the learning rate from 0.1 of the peak to the peak value within the first 10% of total iterations, followed by a decay to 0.1 of the peak using a cosine schedule.

I Algorithms for One-Hop Searching

We now introduce the Algorithm 4 used for searching the best one-hop hypothesis with the tail among all entities in the observation set to explain the observations.

Algorithm 4 One-Hop-Search

Input Observation set O
Output Hypothesis $bestHypothesis$
$candidates \leftarrow \{(h, r, t) \in \mathcal{R}_\text{train} | t \in O\}$
$bestJaccard \leftarrow 0$
$bestHypothesis \leftarrow$ Null
for $(h, r, t) \in candidates$ **do**
  $H \leftarrow$ the one-hop hypothesis consisting of edge (h, r, t)
  $nowJaccard \leftarrow \texttt{Jaccard}([\![H]\!]_{\mathcal{G}_\text{train}}, A)$
  if $nowJaccard > bestJaccard$ **then**
    $bestJaccard \leftarrow nowJaccard$
    $bestHypothesis \leftarrow H$
  end if
end for
return $bestHypothesis$

J Case Studies

Explore Table 9, 10 and 11 for concrete examples generated by various abductive reasoning methods, namely search, generative model with supervised training, and generative model with supervised training incorporating RLF-KG.

Dataset	Model	1p	2p	2i	3i	ip	pi	2u	up	2in	3in	pni	pin	inp	Ave.
FB15k-237	Enc.-Dec.	0.342	0.506	0.595	0.602	0.570	0.598	0.850	0.571	0.652	0.641	0.650	0.655	0.599	0.602
	RLF-KG (J)	0.721	0.643	0.562	0.480	0.364	0.475	0.769	0.431	0.543	0.499	0.513	0.518	0.370	0.530
	RLF-KG (J+S)	0.591	0.583	0.577	0.531	0.447	0.520	0.820	0.505	0.602	0.563	0.571	0.595	0.484	0.568
	Dec.-Only	0.287	0.481	0.615	0.623	0.599	0.626	0.847	0.574	0.680	0.656	0.675	0.677	0.636	0.614
	RLF-KG (J)	0.344	0.445	0.675	0.585	0.537	0.638	0.853	0.512	0.696	0.575	0.647	0.688	0.574	0.598
	RLF-KG (J+S)	0.303	0.380	0.692	0.607	0.565	0.671	0.857	0.506	0.727	0.600	0.676	0.734	0.634	0.612
WN18RR	Enc.-Dec.	0.375	0.452	0.591	0.555	0.437	0.585	0.835	0.685	0.586	0.516	0.561	0.549	0.530	0.558
	RLF-KG (J)	0.455	0.468	0.563	0.562	0.361	0.530	0.810	0.646	0.560	0.530	0.536	0.539	0.465	0.540
	RLF-KG (J+S)	0.443	0.457	0.565	0.572	0.366	0.545	0.814	0.661	0.541	0.553	0.532	0.546	0.491	0.545
	Dec.-Only	0.320	0.443	0.582	0.551	0.486	0.597	0.809	0.696	0.594	0.526	0.575	0.574	0.577	0.564
	RLF-KG (J)	0.400	0.438	0.566	0.491	0.403	0.519	0.839	0.667	0.547	0.450	0.497	0.466	0.450	0.518
	RLF-KG (J+S)	0.375	0.447	0.584	0.499	0.432	0.545	0.825	0.679	0.584	0.477	0.543	0.522	0.507	0.540
DBpedia50	Enc.-Dec.	0.345	0.396	0.570	0.548	0.344	0.576	0.712	0.544	0.474	0.422	0.477	0.488	0.428	0.486
	RLF-KG (J)	0.461	0.424	0.634	0.584	0.361	0.575	0.809	0.579	0.584	0.497	0.544	0.533	0.454	0.541
	RLF-KG (J+S)	0.419	0.410	0.638	0.555	0.373	0.586	0.785	0.579	0.560	0.459	0.536	0.542	0.474	0.532
	Dec.-Only	0.378	0.408	0.559	0.526	0.397	0.568	0.812	0.626	0.480	0.414	0.489	0.494	0.474	0.510
	RLF-KG (J)	0.405	0.411	0.558	0.496	0.376	0.507	0.825	0.621	0.477	0.397	0.468	0.444	0.406	0.492
	RLF-KG (J+S)	0.398	0.415	0.567	0.497	0.383	0.533	0.827	0.630	0.510	0.420	0.484	0.457	0.430	0.504

Table 6: The detailed Smatch performance of various methods.

Dataset	1p	2p	2i	3i	ip	pi	2u	up	2in	3in	pni	pin	inp	Ave.
FB15k-237	0.945	0.340	0.365	0.218	0.184	0.267	0.419	0.185	0.301	0.182	0.245	0.155	0.157	0.305
WN18RR	0.957	0.336	0.420	0.274	0.182	0.275	0.427	0.183	0.323	0.224	0.270	0.155	0.156	0.322
DBpedia	0.991	0.336	0.399	0.259	0.182	0.245	0.441	0.183	0.332	0.226	0.290	0.154	0.155	0.322

Table 7: The detailed Smatch performance of the searching method.

Hyperparam.	Enc.-Dec.			Dec.-Only		
	FB15k-237	WN18RR	DBpedia50	FB15k-237	WN18RR	DBpedia50
Learning rate	2.4e-5	3.1e-5	1.8e-5	0.8e-5	0.8e-5	0.6e-5
Batch size	16384	16384	4096	3072	2048	2048
Minibatch size	512	512	64	96	128	128
Horizon	4096	4096	4096	2048	2048	2048

Table 8: PPO Hyperparamters.

Sample	Interpretation	Companies operating in industries that intersect with Yahoo! but not with IBM.
	Hypothesis	The observations are the $V_?$ such that $\exists V_1, inIndustry(V_1, V_?) \wedge \neg industryOf(IBM, V_1) \wedge industryOf(Yahoo!, V_1)$
	Observation	EMI, Columbia, Viacom, Yahoo!, Bandai, Rank_Organisation, Gannett_Company, NBCUniversal, Pony_Canyon, The_Graham_Holdings_Company, Televisa, Google, Microsoft_Corporation, Munhwa_Broadcasting_Corporation, CBS_Corporation, GMA_Network, Victor_Entertainment, Sony_Music_Entertainment_(Japan)_Inc., Toho_Co.,_Ltd., The_New_York_Times_Company, Star_Cinema, TV5, Avex_Trax, The_Walt_Disney_Company, Metro-Goldwyn-Mayer, Time_Warner, Dell, News_Corporation
Searching	Interpretation	Which companies operate in media industry?
	Hypothesis	The observations are the $V_?$ such that $inIndustry(Media, V_?)$
	Conclusion	Absent: - Google, - Microsoft_Corporation, - Dell
	Jaccard	0.893
	Smatch	0.154
Enc.-Dec.	Interpretation	Companies operating in industries that intersect with Yahoo! but not with Microsoft Corporation.
	Hypothesis	The observations are the $V_?$ such that $\exists V_1, inIndustry(V_1, V_?) \wedge \neg industryOf(Microsoft\_Corporation, V_1) \wedge industryOf(Yahoo!, V_1)$
	Conclusion	Absent: Microsoft_Corporation
	Jaccard	0.964
	Smatch	0.909
+ RLF-KG	Interpretation	Companies operating in industries that intersect with Yahoo! but not with Oracle Corporation.
	Hypothesis	The observations are the $V_?$ such that $\exists V_1, inIndustry(V_1, V_?) \wedge \neg industryOf(Oracle\_Corporation, V_1) \wedge industryOf(Yahoo!, V_1)$
	Concl.	Same
	Jaccard	1.000
	Smatch	0.909

Table 9: Example FB15k-237 Case study 1.

Sample	Interpretation	Locations that adjoin second-level divisions of the United States of America that adjoin Washtenaw County.
	Hypothesis	The observations are the $V_?$ such that $\exists V_1, adjoins(V_1, V_?) \wedge adjoins(Washtenaw\_County, V_1) \wedge secondLevelDivisions(USA, V_1)$
	Observation	Jackson_County, Wayne_County, Washtenaw_County, Macomb_County, Ingham_County
Searching	Interpretation	Locations that adjoin Oakland County.
	Hypothesis	The observations are the $V_?$ such that $adjoins(Oakland\_County, V_?)$
	Conclusion	Absent: - Jackson_County - Ingham_County
	Jaccard	0.600
	Smatch	0.182
Enc.-Dec.	Interpretation	Second-level divisions of the United States of America that adjoin locations that adjoin Oakland County.
	Hypothesis	The observations are the $V_?$ such that $\exists V_1, secondLevelDivisions(USA, V_?) \wedge adjoins(V_1, V_?) \wedge +adjoins(Oakland\_County, V_1)$
	Conclusion	Extra: Oakland_County Absent: Wayne_County
	Jaccard	0.667
	Smatch	0.778
+ RLF-KG	Interpretation	Second-level divisions of the United States of America that adjoin locations contained within Michigan.
	Hypothesis	The observations are the $V_?$ such that $\exists V_1, secondLevelDivisions(USA, V_?) \wedge adjoins(V_1, V_?) \wedge containedIn(Michigan, V_1)$
	Conclusion	Extra: - Oakland_County - Genesee_County
	Jaccard	0.714
	Smatch	0.778

Table 10: FB15k-237 Case study 2.

Ground Truth	Interpretation	Works, except for “Here ’Tis,” that have subsequent works in the jazz genre.
	Hypothesis	The observations are the $V_?$ such that $\exists V_1, subsequentWork(V_1, V_?) \wedge \neg previousWork(Here\_'Tis, V_1) \wedge genre(Jazz, V_1)$
	Observation	Deep,_Deep_Trouble, Good_Dog,_Happy_Man, I_Don’t_Want_to_Be_Your_Friend, Interior_Music, Lee_Morgan_Sextet, Paris_Nights\/New_York_Mornings, Take_the_Box
Searching	Interpretation	Works subsequent to “Closer” (Corinne Bailey Rae song).
	Hypothesis	The observations are the $V_?$ such that $subsequentWork(Closer\_(Corinne\_Bailey\_Rae\_song), V_?)$
	Conclusion	Only Paris_Nights\/New_York_Mornings
	Jaccard	0.143
	Smatch	0.154
Enc.-Dec.	Interpretation	Works, except for “Lee Morgan Sextet,” that have subsequent works in the jazz genre.
	Hypothesis	The observations are the $V_?$ such that $\exists V_1, subsequentWork(V_1, V_?) \wedge \neg previousWork(Lee\_Morgan\_Sextet, V_1) \wedge genre(Jazz, V_1)$
	Conclusion	Extra: Here_’Tis Absent: Lee_Morgan_Sextet
	Jaccard	0.750
	Smatch	0.909
+ RLF-KG	Interpretation	Works that have subsequent works in the jazz genre.
	Hypothesis	The observations are the $V_?$ such that $\exists V_1, subsequentWork(V_1, V_?) \wedge genre(Jazz, V_1)$
	Conclusion	Extra: Here_’Tis
	Jaccard	0.875
	Smatch	0.400

Table 11: DBpedia50 Case study.