

# MLV Lab AGI Study

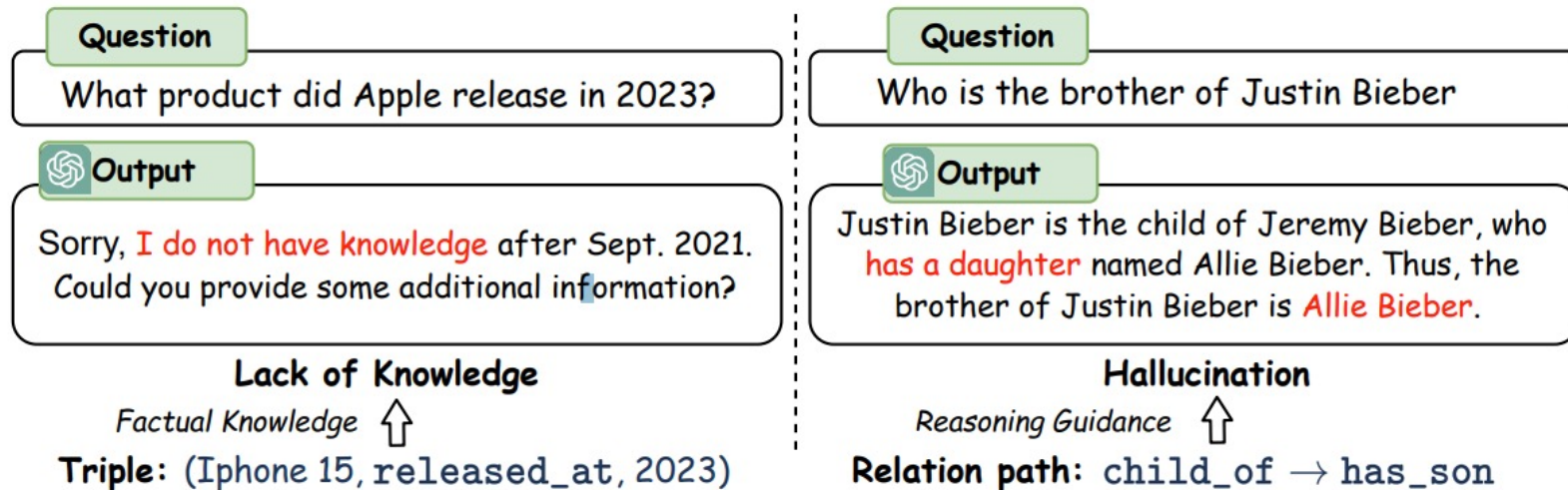
## **Reasoning on Graphs: Faithful and Interpretable Large Language Model Reasoning**

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# Introduction

- LLM은 QA task에서 지식이 부족하거나 hallucination을 하는 문제가 있음



- Knowledge Graphs를 이용하면 이 문제들을 해결할 수 있음

# Introduction

- 이전의 LLM 기반 KGQA 접근법들은
  - 논리적인 query를 만들지 못하거나 (semantic parsing methods)
  - 그래프의 구조적 정보를 활용하지 못함 (retrieval-augmented methods)
- 신뢰 가능하고 해석 가능한 추론을 위해 LLM이 직접적으로 KG에서 추론하는 것이 중요
- Reasoning on Graphs (RoG) 방법론 제안

# Introduction

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- RoG -> planning-retrieval-reasoning framework
  1. Planning module
    - 신뢰 가능한 plans로 사용하기 위해 relation paths를 만듦
  2. Retrieval-reasoning module
    - 유효한 reasoning paths를 retrieve
    - reasoning paths를 기반으로 추론

# Preliminary

- Relation Paths

- sequence of relations:  $z = \{r_1, \dots, r_l\}$   
where  $r_i \in \mathcal{R}$  denotes the  $i$ -th relation in the path

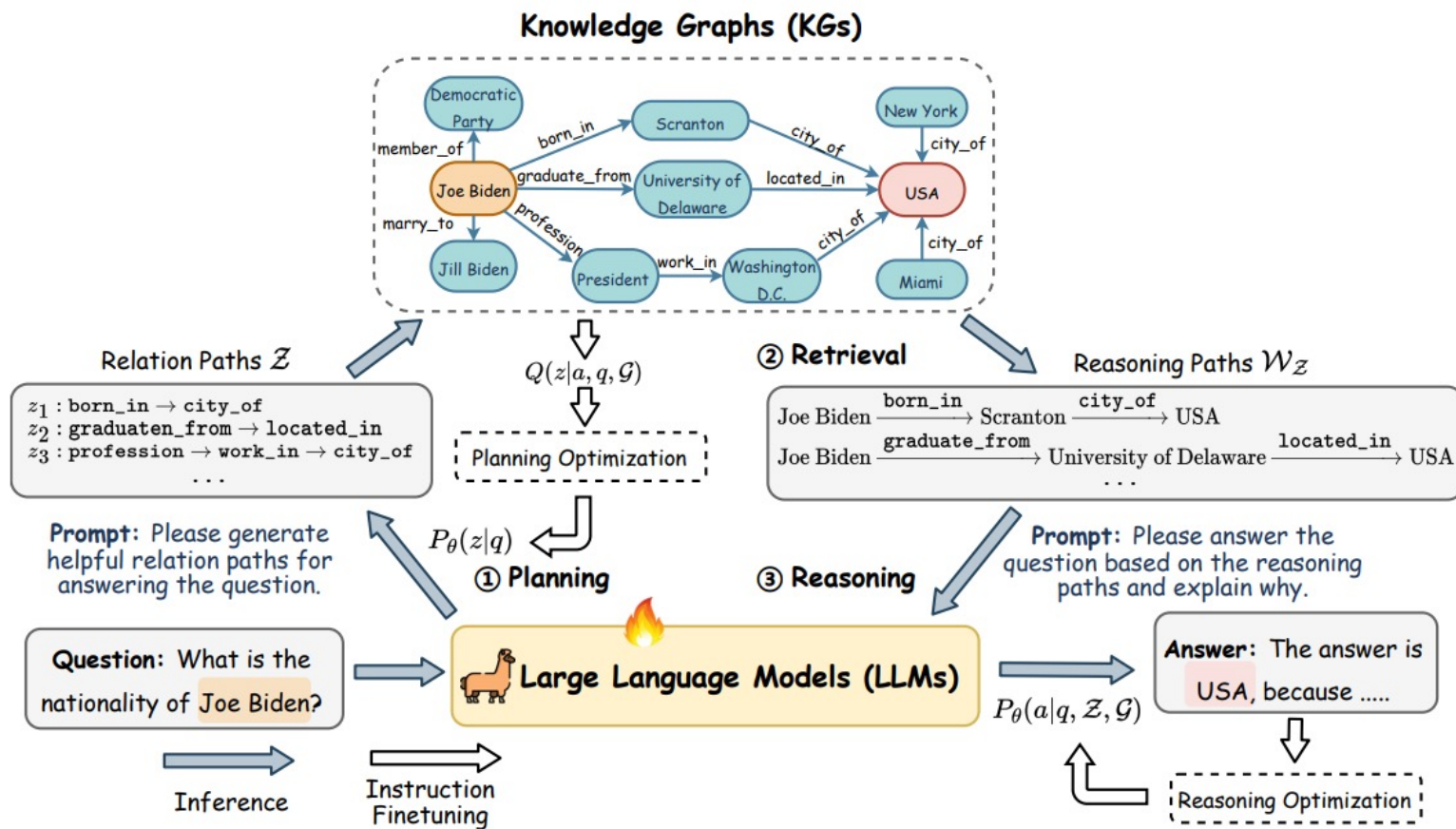
- Reasoning Paths

- instances of a relation path  $z$  in KGs:

$$w_z = e_0 \xrightarrow{r_1} e_1 \xrightarrow{r_2} \dots \xrightarrow{r_l} e_l$$

where  $e_i \in \mathcal{E}$  denotes the  $i$ -th entity

# Approach



# Approach

**Planning:** generates a relation path as the plan

- “Who is the child of Alice?” 이라는 질문이 들어오면,  
 $z = \text{marry\_to} \rightarrow \text{father\_of}$  라는 relation path를 찾는 것이 목표
- Relation path는 다음과 같은 plan을 표현
  - Alice 와 결혼한 사람을 찾음 (marry\_to)
  - 그 사람의 아이를 찾음 (father\_of)

# Approach

**Retrieval:** retrieve a reasoning path from KGs

- Retrieve  $w_z = \text{Alice} \xrightarrow{\text{marry-to}} \text{Bob} \xrightarrow{\text{father-of}} \text{Charile}$

**Reasoning:** answer the question based on the reasoning path

- “Charlie”



# Approach

- RoG as an optimization problem: maximize the probability

$$P_{\theta}(a|q, \mathcal{G}) = \sum_{z \in \mathcal{Z}} P_{\theta}(a|q, z, \mathcal{G}) P_{\theta}(z|q)$$

- $z$ : relation paths generated by LLMs
- $q, a$ : question & answer
- $\theta$ : parameters of LLMs
- $\mathcal{G}$ : KGs
- $Q(z)$ : 신뢰 가능한 relation paths의 posterior distribution

# Approach

- Maximize probability  $\rightarrow$  Maximize the evidence lower bound (ELBO)

$$P_{\theta}(a|q, G) = \sum_{z \in \mathcal{Z}} P_{\theta}(a|q, z, G) \cdot P_{\theta}(z|q)$$

$$\begin{aligned} \log P_{\theta}(a|q, G) &= \log \sum_{z \in \mathcal{Z}} P_{\theta}(a|q, z, G) \cdot P_{\theta}(z|q) \\ &= \log \sum_{z \in \mathcal{Z}} P_{\theta}(a|q, z, G) \cdot P_{\theta}(z|q) \cdot \frac{Q(z)}{Q(z)} \\ &= \log \sum_{z \in \mathcal{Z}} Q(z) \cdot \frac{P_{\theta}(a|q, z, G) \cdot P_{\theta}(z|q)}{Q(z)} \\ &\geq \sum_{z \in \mathcal{Z}} Q(z) \log \frac{P_{\theta}(a|q, z, G) \cdot P_{\theta}(z|q)}{Q(z)} \end{aligned}$$

$$\begin{aligned} &\sum_{z \in \mathcal{Z}} \left[ Q(z) \log P_{\theta}(a|q, z, G) \cdot P_{\theta}(z|q) - Q(z) \log Q(z) \right] \\ &= \sum_{z \in \mathcal{Z}} \left[ Q(z) \log P_{\theta}(a|q, z, G) - Q(z) \log \frac{Q(z)}{P_{\theta}(z|q)} \right] \\ &= \underbrace{\mathbb{E}_{z \sim Q(z)} \log P_{\theta}(a|q, z, G)}_{\textcircled{2}} - \underbrace{KL(Q(z) \| P_{\theta}(z|q))}_{\textcircled{1}} \end{aligned}$$

# Approach

- Optimization problem

$$\log P_\theta(a|q, G) \geq \underbrace{\mathbb{E}_{z \sim Q(z)} \log P_\theta(a|q, z, G)}_{\textcircled{2}} - \underbrace{KL(Q(z) \| P_\theta(z|q))}_{\textcircled{1}}$$

1. posterior 와 prior 간 KL divergence 최소화:  
LLMs 이 신뢰 가능한 relation paths를 만들도록 유도 (planning)
2. 질문과 relation paths, KG로 정답을 만들 확률의 평균을 최대화:  
relation paths 와 KGs를 기반으로 정답을 찾도록 유도 (retrieval-reasoning)

# Approach

- (1) = Planning Optimization

$$Q(z) \simeq Q(z|a, q, \mathcal{G}) = \begin{cases} 1, \exists w_z(e_q, e_a) \in \mathcal{G}, \\ 0, \text{else.} \end{cases}$$

$$\begin{aligned} \mathcal{L}_{\text{plan}} &= D_{\text{KL}}(Q(z) \| P_{\theta}(z|q)) = D_{\text{KL}}(Q(z|a, q, \mathcal{G}) \| P_{\theta}(z|q)) \\ &= \mathbb{E}_{z \sim Q(z|a, q, \mathcal{G})} Q(z|a, q, \mathcal{G}) [\log Q(z|a, q, \mathcal{G}) - \log P_{\theta}(z|q)] \\ &= -\mathbb{E}_{z \sim Q(z|a, q, \mathcal{G})} Q(z|a, q, \mathcal{G}) \log P_{\theta}(z|q) + \text{CONST} \\ &= - \sum_{z \in Q(z|a, q, \mathcal{G})} \log P_{\theta}(z|q). \end{aligned}$$

# Approach

- (2) = Retrieval-reasoning Optimization

$$P_{\theta}(a|q, \mathcal{Z}, \mathcal{G}) = \prod_{z \in \mathcal{Z}} P_{\theta}(a|q, z, \mathcal{G})$$

$$\mathcal{L}_{\text{reason}} = \mathbb{E}_{z \sim Q(z|a, q, \mathcal{G})} [\log P_{\theta}(a|q, z, \mathcal{G})] = \log P_{\theta}(a|q, \mathcal{Z}_K, \mathcal{G})$$

# Approach

- Optimization problem

$$\mathcal{L} = \underbrace{\log P_{\theta}(a|q, \mathcal{Z}_K, \mathcal{G})}_{\text{Retrieval-reasoning}} + \underbrace{\sum_{z \in Q(z|a, q, \mathcal{G})} \log P_{\theta}(z|q)}_{\text{Planning}}$$

- Instruction-tuning tasks로 LLM을 학습시킴

# Approach

## Planning Module

- 질문을 보고 relation paths를 만듦

- Prompt

### Planning Prompt Template

Please generate a valid relation path that can be helpful for answering the following question:  
<Question>

- Output

$$z = \langle \text{PATH} \rangle r_1 \langle \text{SEP} \rangle r_2 \langle \text{SEP} \rangle \dots \langle \text{SEP} \rangle r_l \langle / \text{PATH} \rangle$$

# Approach

## Retrieval-Reasoning Module

- KG로부터 question entities  $e_q$ 에서 answer entities  $e_a$ 로 가는 reasoning path  $w_z$ 를 찾음

$$\mathcal{W}_z = \{w_z(e_q, e_*) | w_z(e_q, e_*) = e_q \xrightarrow{r_1} e_1 \xrightarrow{r_2} \dots \xrightarrow{r_l} e_{a*}, w_z(e_q, e_*) \in \mathcal{G}\}$$

- Breadth-first search



# Approach

- Retrieval algorithm

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**Algorithm 1:** Retrieve reasoning paths based on relation paths

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**Input:** Question  $q$ , relation path  $z = \{r_1, r_2, \dots, r_l\}$ , KG  $\mathcal{G}$ .

**Output:** Reasoning paths  $\mathcal{W}_z$ .

```
1  $\mathcal{W}_z \leftarrow \emptyset$ ;  
2  $\mathcal{Q} \leftarrow \text{Queue}()$ ;  
3 foreach  $e_q \in \mathcal{T}_q$  do  
4    $\mathcal{Q}.\text{append}((e_q, []))$ ; // Initialize queue with question entities.  
5 end  
6 while  $\mathcal{Q} \neq \emptyset$  do  
7    $(s, w_z) \leftarrow \mathcal{Q}.\text{pop}()$ ;  
8   if  $\text{len}(w_z) = \text{len}(z)$  then  
9      $\mathcal{W}_z.\text{append}(w_z)$ ;  
10  end  
11  if  $\text{len}(w_z) < \text{len}(z)$  then  
12     $r \leftarrow z[\text{len}(w_z) + 1]$ ; // Get relation for next step.  
13    foreach  $(s, r', t) \in \mathcal{G}$  do  
14      if  $r' = r$  then  
15         $w'_z.\text{append}((s, r, t))$ ; // Expand the reasoning path.  
16         $\mathcal{Q}.\text{append}((t, w'_z))$ ;  
17      end  
18    end  
19  end  
20 end  
21 return  $\mathcal{W}_z$ ;
```

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# Approach

## Retrieval-Reasoning Module

- 질문과 reasoning paths를 받아 정답을 냄
  - Prompt

### Reasoning Prompt Template

Based on the reasoning paths, please answer the given question. Please keep the answer as simple as possible and return all the possible answers as a list.

Reasoning Paths:

<Reasoning Paths>

Question:

<Question>

# Experiment

## Research Questions

- RQ1: RoG가 KGQA tasks에서 SOTA 성능을 달성했는가?
- RQ2: RoG의 planning module이 다른 LLM에 사용되어 성능을 개선시킬 수 있는가?
- RQ3: RoG가 다른 KG에 transfer 될 수 있는가?
- RQ4: RoG가 실제로 신뢰 가능하고 해석 가능한 추론을 하는가?

# Experiment

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## Dataset

- KGQA dataset: WebQuestionSP, WebQuestions
- KG: Freebase

## Implementations

- LLM backbone: LLaMA2-Chat-7B
- top-3 relation paths를 사용

# Experiment: RQ1

Type	Methods	WebQSP		CWQ	
		Hits@1	F1	Hits@1	F1
Embedding	KV-Mem (Miller et al., 2016)	46.7	34.5	18.4	15.7
	EmbedKGQA (Saxena et al., 2020)	66.6	-	45.9	-
	NSM (He et al., 2021)	68.7	62.8	47.6	42.4
	TransferNet (Shi et al., 2021)	71.4	-	48.6	-
	KGT5 Saxena et al. (2022)	56.1	-	36.5	-
Retrieval	GraftNet (Sun et al., 2018)	66.4	60.4	36.8	32.7
	PullNet (Sun et al., 2019)	68.1	-	45.9	-
	SR+NSM (Zhang et al., 2022)	68.9	64.1	50.2	47.1
	SR+NSM+E2E (Zhang et al., 2022)	69.5	64.1	49.3	46.3
Semantic Parsing	SPARQL (Sun et al., 2020)	-	-	31.6	-
	QGG (Lan & Jiang, 2020)	73.0	73.8	36.9	37.4
	ArcaneQA (Gu & Su, 2022)	-	75.3	-	-
	RnG-KBQA (Ye et al., 2022)	-	76.2	-	-
LLMs	Flan-T5-xl (Chung et al., 2022)	31.0	-	14.7	-
	Alpaca-7B (Taori et al., 2023)	51.8	-	27.4	-
	LLaMA2-Chat-7B (Touvron et al., 2023)	64.4	-	34.6	-
	ChatGPT	66.8	-	39.9	-
	ChatGPT+CoT	75.6	-	48.9	-
LLMs+KGs	KD-CoT (Wang et al., 2023b)	68.6	52.5	55.7	-
	UniKGQA (Jiang et al., 2022)	77.2	72.2	51.2	49.1
	DECAF (DPR+FiD-3B) (Yu et al., 2022a)	82.1	<b>78.8</b>	-	-
	RoG	<b>85.7</b>	70.8	<b>62.6</b>	<b>56.2</b>

?

# Experiment: RQ1

- Ablation Study

Method	WebQSP			CWQ		
	Precision	Recall	F1	Precision	Recall	F1
RoG	<b>74.77</b>	75.84	<b>70.81</b>	<b>57.69</b>	58.19	<b>56.17</b>
RoG w/o planning	57.26	50.16	49.69	35.35	34.77	33.76
RoG w/o reasoning	46.90	<b>79.85</b>	49.56	18.88	<b>67.89</b>	22.26
RoG w/ random plans	38.66	38.31	35.24	38.99	39.29	37.64
RoG w/ vote reasoning	54.80	60.44	47.96	22.92	47.98	26.52

- Recall은 답의 수가 증가했기 때문에 올랐고,  
Precision은 retrieved paths에 noise가 있기 때문에 떨어짐

# Experiment: RQ2

- Planning module은 그대로 사용하고, reasoning 하는 LLM만 변경

Methods	WebQSP		CWQ	
	Hits@1	Recall	Hits@1	Recall
ChatGPT	66.77	49.27	39.90	35.07
ChatGPT + RoG Planning	<b>81.51</b>	<b>71.60</b>	<b>52.68</b>	<b>48.51</b>
Alpaca-7B	51.78	33.65	27.44	23.62
Alpaca-7B + RoG Planning	<b>56.16</b>	<b>74.20</b>	<b>44.04</b>	<b>38.46</b>
LLaMA2-Chat-7B	64.37	44.61	34.60	29.91
LLaMA2-Chat-7B + RoG Planning	<b>74.20</b>	<b>56.16</b>	<b>56.41</b>	<b>51.99</b>
Flan-T5-xl	30.95	17.08	14.69	12.25
Flan-T5-xl + RoG Planning	<b>67.87</b>	<b>44.93</b>	<b>37.81</b>	<b>32.57</b>

# Experiment: RQ3

- Transferability to other KGs
  - MetaQA-3hop dataset, Wiki-Movies KGs 사용

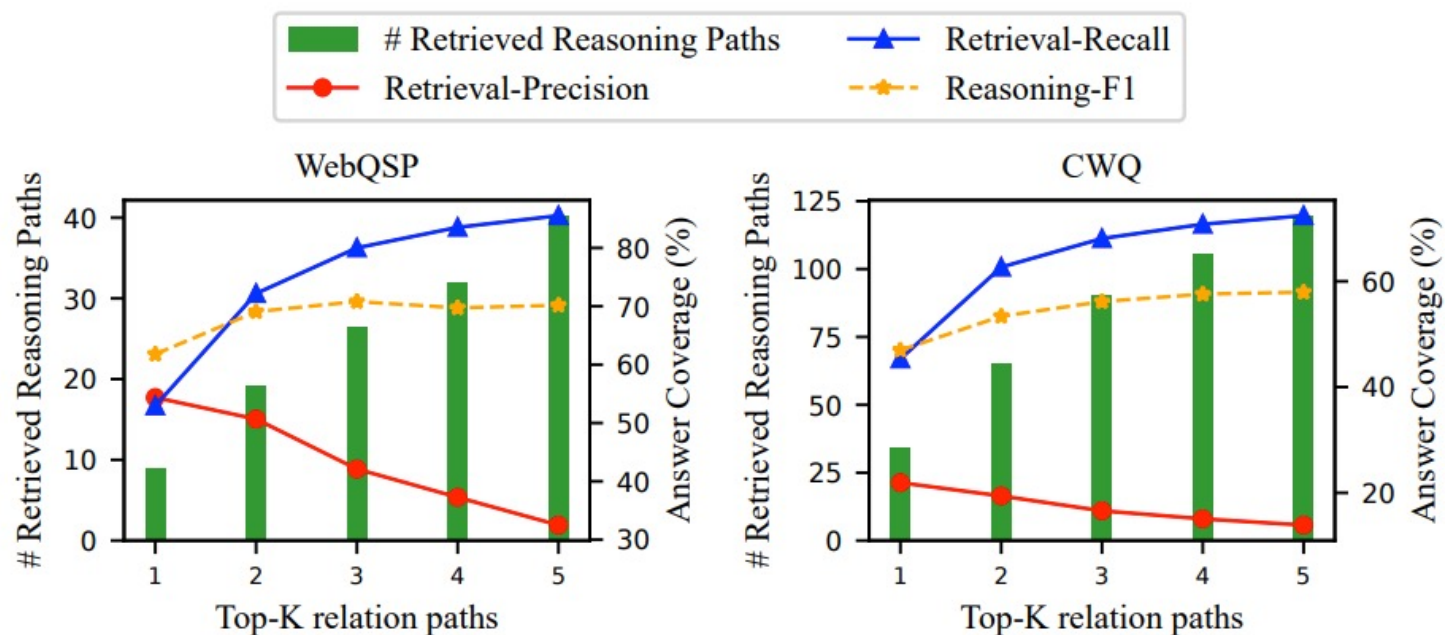
Strategies	MetaQA-3hop	
	Hits@1	F1
RoG (train from scratch)	84.81	41.32
RoG (transfer from Freebase)	<b>88.98</b>	<b>50.68</b>

1. 1000 samples로 RoG 학습
2. 추가적으로 Freebase(다른 KG)에 기반한 학습



# Experiment: RQ4

- 신뢰 가능성



- Retrieved Reasoning paths가 많아질수록 Recall이 증가 -> 신뢰 가능

# Experiment: RQ4

- 해석 가능성

Question	What type of government is used in the country with Northern District?
Answer	Parliamentary system
ChatGPT + CoT	To determine what type of government is used in a country with a Northern District, <b>we need more specific information</b> . The term "Northern District" does not specify the name of any particular country or provide enough context to identify its government type. <b>Could you please provide additional details or clarify the specific country you are referring to?</b>
Reasoning Paths	Northern District → location.administrative_division.first_level_division_of → Israel → government.form_of_government.countries → <b>Parliamentary system</b>
RoG	<p>The type of government used in the country with the Northern District is a <b>Parliamentary system</b>.</p> <p>Explanations:</p> <ol style="list-style-type: none"><li>1. Northern District → location.administrative_division.first_level_division_of → Israel: The Northern District is a part of Israel.</li><li>2. Israel → government.form_of_government.countries → Parliamentary system: Israel has a Parliamentary system of government.</li></ol> <p>So, by <u>following the reasoning paths provided</u>, we can conclude that the country with the Northern District, which is Israel, uses a Parliamentary system of government.</p>

# Experiment: RQ4

- Hallucination

Question	Where is the home stadium of the team who won the 1946 World Series championship?
Answer	Busch Stadium
ChatGPT + CoT	<p>Step 1: Identify the team that won the 1946 World Series championship. The team that won the 1946 World Series championship was the St. Louis Cardinals.</p> <p>Step 2: Determine the home stadium of the St. Louis Cardinals during that time. The St. Louis Cardinals' home stadium during the 1946 season was <b>Sportsman's Park</b>.</p> <p>Therefore, the possible answer to the question "Where is the home stadium of the team who won the 1946 World Series championship?" is: - <b>Sportsman's Park</b>.</p>
Reasoning Paths	<p>1946 World Series → sports.sports_team.championships → St. Louis Cardinals → sports.sports_team.arena_stadium → <b>Busch Stadium</b></p> <p>1946 World Series → sports.sports_team.championships → St. Louis Cardinals → sports.sports_team.arena_stadium → <b>Roger Dean Stadium</b></p>
RoG	<p>Based on the reasoning paths provided, the home stadium of the team who won the 1946 World Series championship is <b>Busch Stadium</b>. This conclusion is based on the following path:</p> <p><b>1. 1946 World Series → sports.sports_team.championships → St. Louis Cardinals → sports.sports_team.arena_stadium → Busch Stadium</b></p> <p>The reasoning path leads us to the St. Louis Cardinals as the team that won the 1946 World Series, and Busch Stadium is the stadium associated with the St. Louis Cardinals. Therefore, <b>Busch Stadium</b> is the home stadium of the team that won the 1946 World Series championship.</p>

# Conclusion

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- Reasoning on Graphs (RoG) method
  - LLM이 KG를 이용하여 신뢰 가능하고 해석 가능한 추론을 함
  - Hallucination과 지식 부족의 문제를 해결
  - 다른 LLM에도 쉽게 적용 가능함

# Questions?

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- Thanks for listening!