CS 957, System-2 AI Reasoning in Knowledge Graphs Through LLMs

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Reasoning on Graphs: Faithful and Interpretable Large Language Model Reasoning

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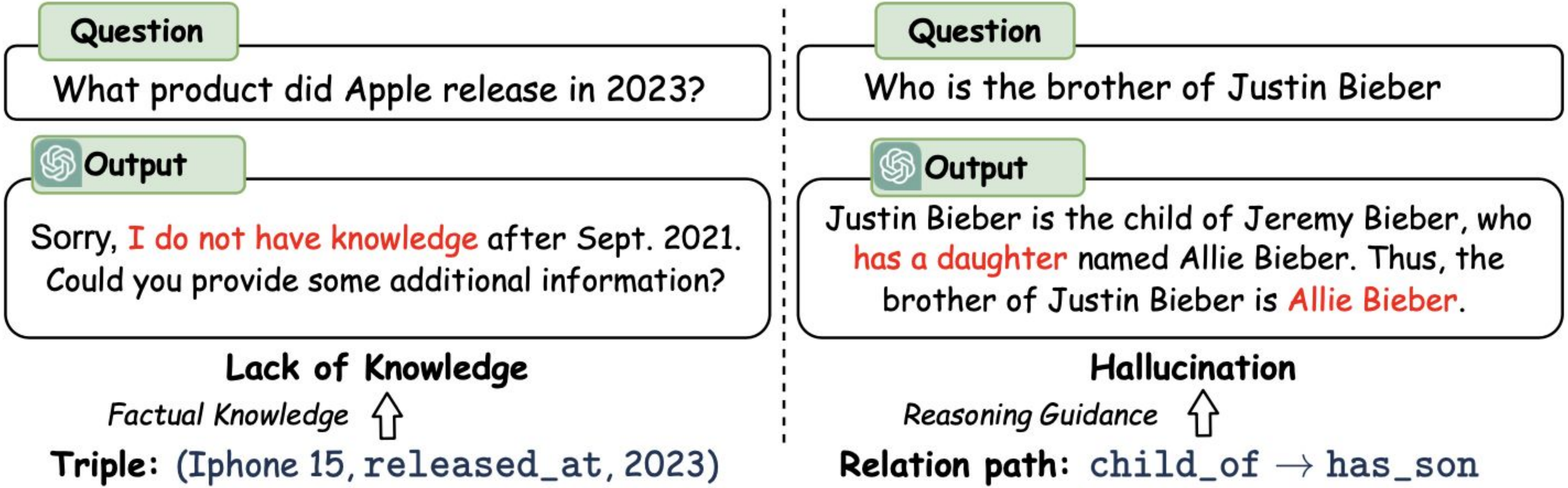
LLMs hallucinate in Question Answering



Let’s brainstorm

Suppose we want to use LLM for KGQA.

How can this be done?

Two Separate Strategies

1. **Semantic parsing** methods (Lan & Jiang, 2020; Ye et al., 2022): use LLMs to convert questions into logical queries that are executed on KGs.

2. **Retrieval-augmented methods** (Li et al., 2023; Jiang et al., 2023): retrieve triples from KGs as knowledge context and uses LLMs to obtain the final answers.

Challenges

How to retrieve relevant information from the KG?

LLM does not have any idea about the semantic of relations in the KG. How to define them for the LLM?

How to leverage relevant structural information in the KG?

Preliminaries and Notation

Knowledge Graphs (KGs) contain abundant factual knowledge in the form of a set of triples: $\mathcal{G} = \{(e, r, e') | e, e' \in \mathcal{E}, r \in \mathcal{R}\}$, where $\mathcal{E}$ and $\mathcal{R}$ denote the set of entities and relations, respectively.

Relation Paths are a sequence of relations: $z = \{r_1, r_2, \ldots, r_l\}$, where $r_i \in \mathcal{R}$ denotes the i-th relation in the path and l denotes the length of the path.

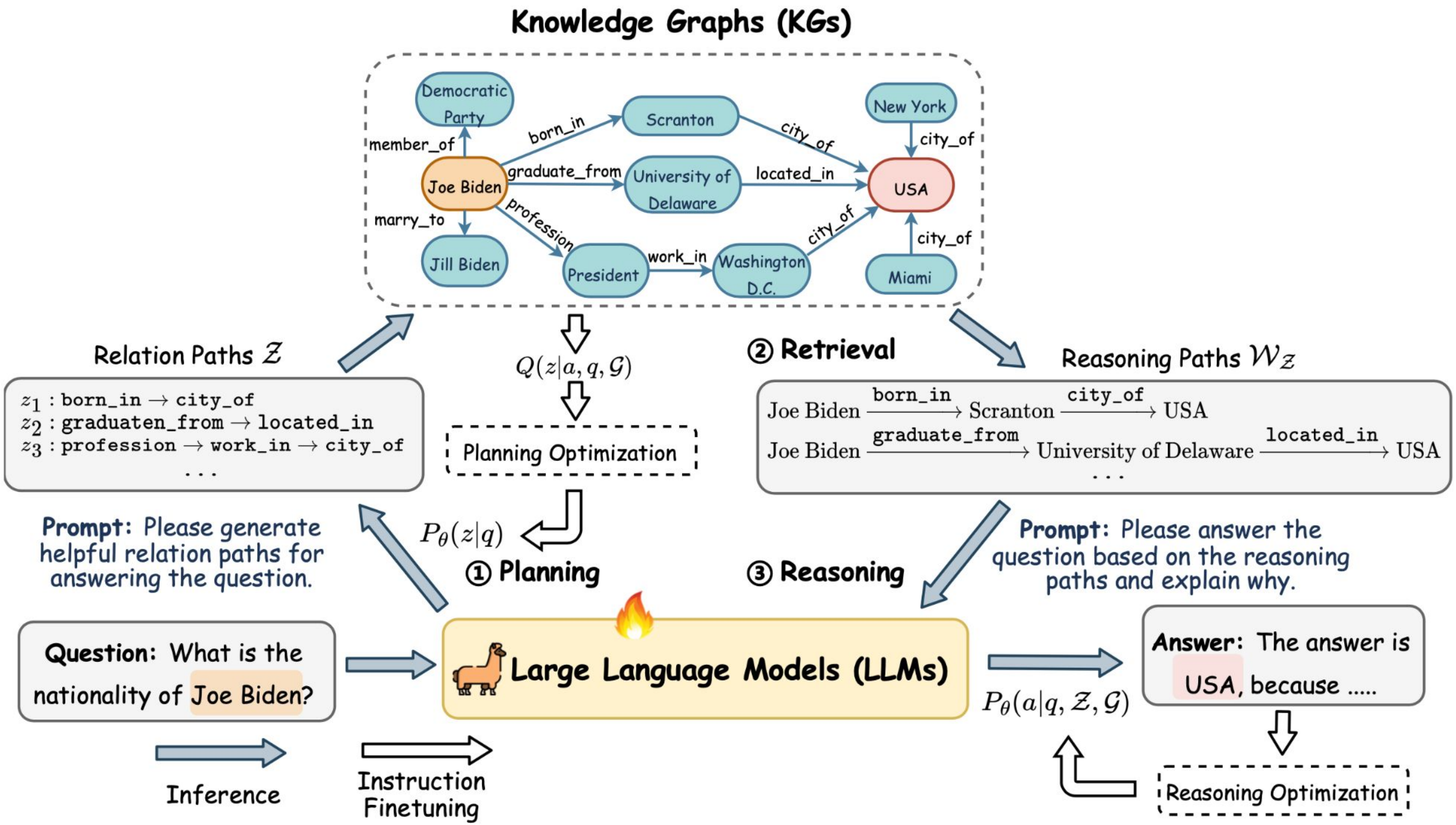
Reasoning Paths are the instances of a relation path z in KGs: $w_z = e_0 \xrightarrow{r_1} e_1 \xrightarrow{r_2} \ldots \xrightarrow{r_l} e_l$, where $e_i \in \mathcal{E}$ denotes the i-th entity and r_i denotes the i-th relation in the relation path z.

Example 1. Given a relation path: $z = \texttt{marry\_to} \rightarrow \texttt{father\_of}$, a reasoning path instance could be: $w_z = \text{Alice} \xrightarrow{\texttt{marry\_to}} \text{Bob} \xrightarrow{\texttt{father\_of}} \text{Charlie}$, which denotes "Alice" is married to "Bob" and "Bob" is the father of "Charlie".

Formal Definition of KGQA

Knowledge Graph Question Answering (KGQA) is a typical reasoning task based on KGs. Given a natural language question q and a KG $\mathcal{G}$, the task aims to design a function f to predict answers $a \in \mathcal{A}_q$ based on knowledge from $\mathcal{G}$, i.e., $a = f(q, \mathcal{G})$. Following previous works (Sun et al., 2019; Jiang et al., 2022), we assume the entities $e_q \in \mathcal{T}_q$ mentioned in q and answers $a \in \mathcal{A}_q$ are labeled and linked to the corresponding entities in $\mathcal{G}$, i.e., $\mathcal{T}_q, \mathcal{A}_q \subseteq \mathcal{E}$.

Method Overview



Planning-Retrieval-Reasoning Framework

Example 2. Given a question "Who is the child of Alice", we can generate a relation path as the plan: $z = \texttt{marry\_to} \rightarrow \texttt{father\_of}$. This relation path expresses the plan: 1) find the person that "Alice" is married to; 2) find the child of that person. We can execute the plan (relation path) by retrieving a reasoning path from KGs as: $w_z = \text{Alice} \xrightarrow{\texttt{marry\_to}} \text{Bob} \xrightarrow{\texttt{father\_of}} \text{Charlie}$. Finally, we can answer the question based on the reasoning path, which is "Charlie".

Solving the Problem as “Maximum Likelihood Estimation” (MLE)

What are the data to feed into MLE?

What are the parameters to fit using MLE?

Any latent variable?

Relation Path as the Latent Variable

How to go about maximizing the likelihood when there are latent variables?

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

Evidence Lower Bound (ELBO)

$$\ln p_\theta(x) \geq \mathbb{E}_{z \sim q_\phi(\cdot|x)} \left[\ln \frac{p_\theta(x, z)}{q_\phi(z|x)} \right]$$

Use Jensen's inequality to prove:

$$\ln p_\theta(x) = \ln \mathbb{E}_{z \sim q_\phi(\cdot|x)} \left[\frac{p_\theta(x, z)}{q_\phi(z|x)} \right] \geq \mathbb{E}_{z \sim q_\phi(\cdot|x)} \left[\ln \frac{p_\theta(x, z)}{q_\phi(z|x)} \right]$$

ELBO Bound in KGQA

$$\log P(a|q,\mathcal{G}) \geq \mathbb{E}_{z\sim Q(z)}[\log P_\theta(a|q,z,\mathcal{G})] - D_{\mathrm{KL}}(Q(z)\|P_\theta(z|q)),$$

where $Q(z)$ denotes the posterior distribution of faithful relation paths grounded by KGs.

What is Q(z)?

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

where we assume a uniform distribution over all valid relation paths $\mathcal{Z}$, and $\exists w_z(e_q, e_a) \in \mathcal{G}$ denote the existence of a path instance connecting the question e_q and answer e_a entities in $\mathcal{G}$. Therefore,

Computing the KL Divergence

$$\mathcal{L}_{\text{plan}} = D_{\text{KL}}(Q(z) \| P_\theta(z|q)) = D_{\text{KL}}(Q(z|a, q, \mathcal{G}) \| P_\theta(z|q)) \simeq -\frac{1}{|\mathcal{Z}^*|} \sum_{z \in \mathcal{Z}^*} \log P_\theta(z|q),$$

where we use the shortest paths $\mathcal{Z}^* \subseteq \mathcal{Z}$ between e_q and e_a in KGs as supervision signals

Optimizing the ELBO

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

$$\mathcal{L} = \log \underbrace{P_\theta(a|q,\mathcal{Z}_K^*,\mathcal{G})}_{\text{Retrieval-reasoning}} + \underbrace{\frac{1}{|\mathcal{Z}^*|}\sum_{z\in Z^*} \log P_\theta(z|q)}_{\text{Planning}}.$$

Planning Module

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

$$z = \texttt{<PATH>}\, r_1\, \texttt{<SEP>}\, r_2\, \texttt{<SEP>} \ldots \texttt{<SEP>}\, r_l\, \texttt{</PATH>}$$

$$\arg\max_{\theta} \frac{1}{|\mathcal{Z}^*|} \sum_{z \in \mathcal{Z}^*} \log P_\theta(z|q) = \frac{1}{|\mathcal{Z}^*|} \sum_{z \in \mathcal{Z}^*} \log \prod_{i=1}^{|z|} P_\theta(r_i | r_{<i}, q),$$

Retrieval-Reasoning Module

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

$$\arg\max_\theta \log P_\theta(a|q, \mathcal{Z}_K^*, \mathcal{G}) = \log \sum_{z \in \mathcal{Z}_K^*} \sum_{w_z \in \mathcal{W}_z} \prod_{i=1}^{|a|} P_\theta(t_i | t_{<i}, q, w_z),$$

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>`

Planning Examples

Question	Top-3 Relation Paths
what does jamaican people speak?	z_1 : location.country.languages_spoken z_2 : language.human_language.countries_spoken_in z_3 : location.country.official_language
where is jamarcus russell from?	z_1 : location.location.people_born_here z_2 : people.person.place_of_birth z_3 : sports.sports_league_draft_pick.player → sports.sports_league_draft_pick.location
where did edgar allan poe died?	z_1 : people.deceased_person.place_of_death z_2 : people.cause_of_death.people z_3 : people.person.place_of_birth
what highschool did harper lee go to?	z_1 : people.person.education → education.educational_institution.students_graduates z_2 : education.education.student → education.educational_institution.students_graduates z_3 : people.person.education → education.education.institutio

Reasoning Examples

Question	what is my timezone in louisiana?
Answer	Central Time Zone
Reasoning Paths	Louisiana → location.location.partially_containedby → Tangipahoa River → geography.river.origin → Osyka → location.location.time_zones → Central Time Zone Louisiana → location.location.containedby → Alexandria → location.location.containedby → United States of America → location.location.time_zones → Central Time Zone
RoG	Based on the reasoning paths provided, it can be determined that Louisiana is in the Central Time Zone. Here's the explanation: 1. The first reasoning path tells us that Louisiana is partially contained by the Tangipahoa River, which is a geographical feature. However, it doesn't directly mention the time zone. 2. The second reasoning path establishes that Louisiana is contained by Alexandria, which is in turn contained by the United States of America. The United States of America is in the Central Time Zone. Therefore, based on these reasoning paths, the time zone in Louisiana is the Central Time Zone.

Experimental Setting

Datasets: WebQuestionSP (WebQSP) (Yih et al., 2016) and Complex WebQuestions (CWQ) containing up to 4-hop questions.

Freebase as the background knowledge graph, containing ~88 million entities, 20 thousand relations, and 126 million triples.

Hits@n: the count of how many positive triples are ranked in the top-n positions against a bunch of synthetic negatives.

Results

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	**78.8**	-	-
	RoG	**85.7**	70.8	**62.6**	**56.2**

Ablation Studies

w/o planning: remove the planning module; perform reasoning without retrieved reasoning paths

w/o reasoning: remove the reasoning module; use all answers from retrieved reasoning

w/ random plans: randomly retrieve reasoning paths from KGs; feed them into the reasoning module

w/ vote reasoning: adopt the majority voting to select top-5 answers from retrieved reasoning paths

Ablation Studies

Method	WebQSP			CWQ		
	Precision	Recall	F1	Precision	Recall	F1
RoG	**74.77**	75.84	**70.81**	**57.69**	58.19	**56.17**
RoG w/o planning	57.26	50.16	49.69	35.35	34.77	33.76
RoG w/o reasoning	46.90	**79.85**	49.56	18.88	**67.89**	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

Planning Module Effect

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

Path Faithfulness