Introduction of my research

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Contents

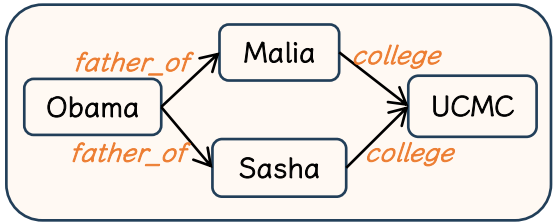
- Backgrounds
  - LMs reasoning over structured environments
  - General pipeline
- Lines of my works
  - Question Decomposition Tree for Answering Complex Questions over Knowledge Bases
  - MarkQA: A large scale KBQA dataset with numerical reasoning
  - QueryAgent: A Reliable and Efficient Reasoning Framework with Environmental Feedback based Self-Correction
  - Call me when necessary: LLMs can Efficiently and Faithfully Reason over Structured Environments

Background

- LMs reasoning over structured environments
- Multi-hop Reasoning task – Question answering
- Structured Environments: **Knowledge graph (base)**, Table, Database, etc

Question: Which college did daughters of Obama go to?

Knowledge graph instances



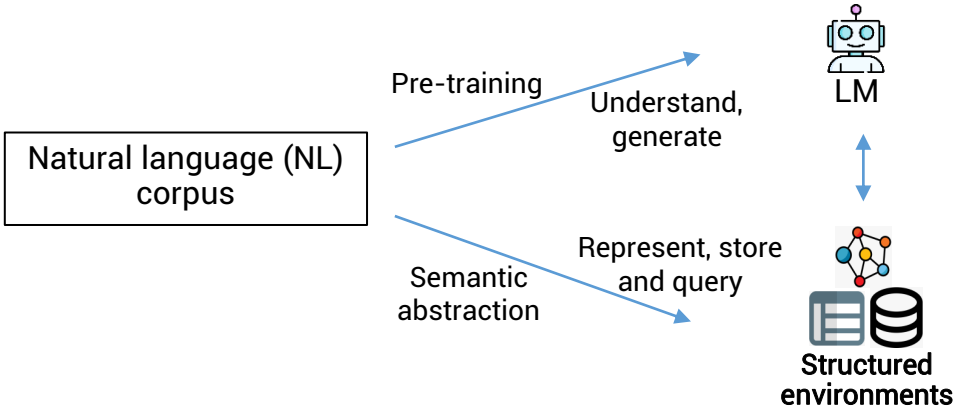
SPARQL Query

```
select ?college where {
Obama father_of ?daughter.
?daughter college ?college.
}
```

Answer: UCMC

Background - Reasoning over structured environments

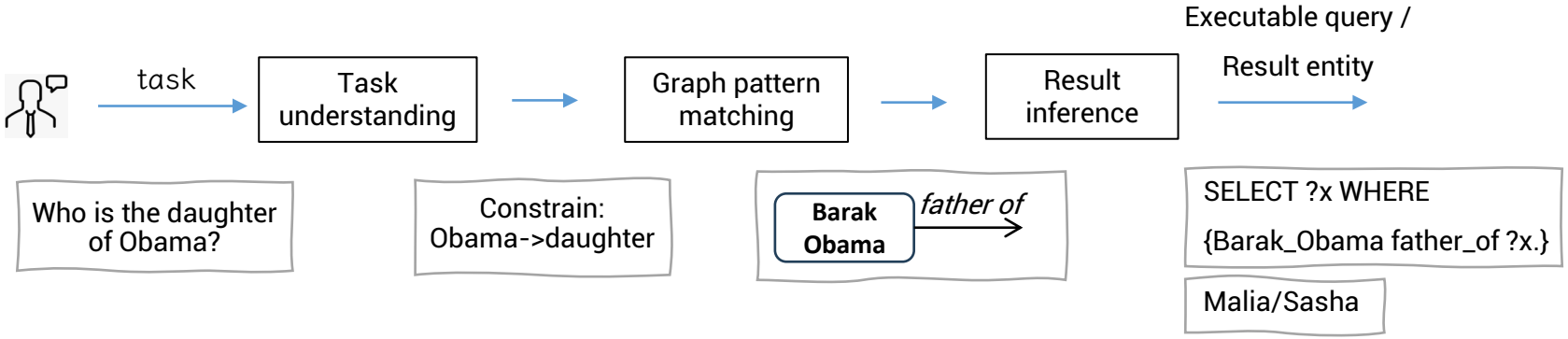
- LMs – Pre-trained from natural language corpus
  - Strong NL understanding and generating ability (by embeddings)
- Structured Environments – abstraction of real-world semantics
  - Representation, store and query of semantics (by **schemas**)
- Challenge
  - **heterogeneity** between task and environment: LMs may not directly understand **schema representations**
  - **large-scale** environment: Cost of annotation & LMs limited context window size



How to introduce structure information to LMs?
· For PLMs
  i. retrieve schemas with an Encoder
  ii. add candidate schemas to Seq2Seq input
· For LLMs
  i. interact with (explore) the environments

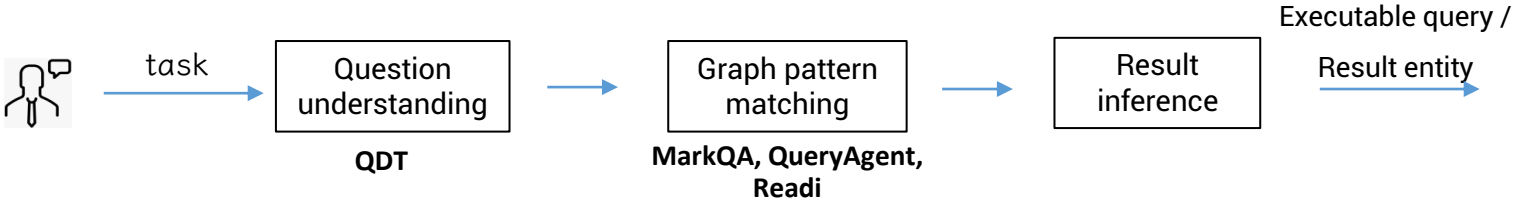
Background – a general pipeline

- Task understanding
  - Complex question → simple constrains and their relations
- Graph pattern matching
  - Entity / relation linking
  - Structure matching (how entities and relations are connected)
- Result inference
  - Semantic parsing (SQL query building)
  - Information retrieval



Background – what I have done ?

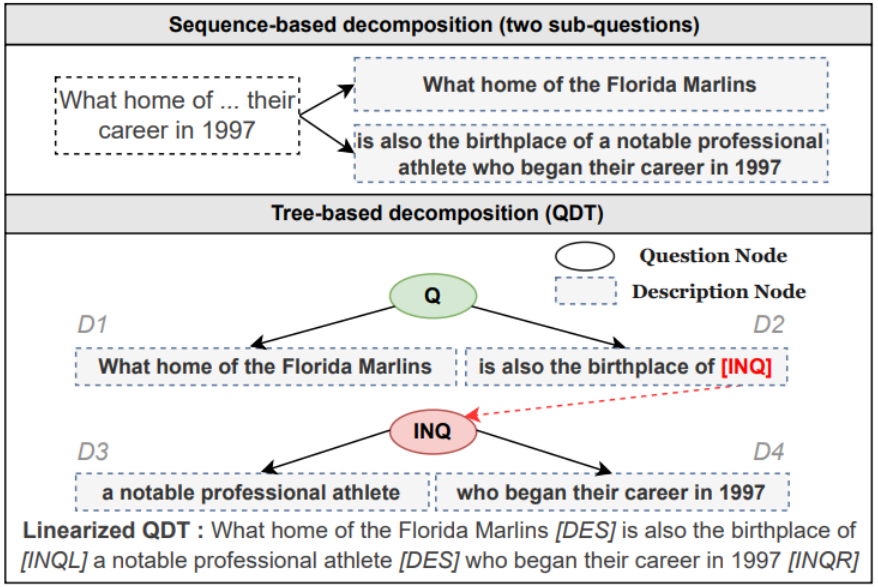
- **Question Decomposition Tree for Answering Complex Questions over Knowledge Bases (AAAI23)**
  - A tree-based decomposition **QDT,** for better **question understanding**
- **MarkQA: A large scale KBQA dataset with numerical reasoning (EMNLP23)**
  - A dataset with complex reasoning structures, for harder **structure matching**
  - Introduce **PyQL function tools** to represent reasoning path
- **QueryAgent: A Reliable and Efficient Reasoning Framework with Environmental Feedback based Self-Correction (Submitted to ACL24)**
  - A LLM-Agent framework using PyQL to **build a query** in a step-by-step manner with correction for **better reasoning**
- **Call Me When Necessary: LLMs can Efficiently and Faithfully Reason over Structured Environments (Submitted to ACL24)**
  - LLMs interaction framework by initially generating a reasoning path, which is instantiated on environments, and edit the path if the instantiation goes wrong



Question Decomposition Tree for Answering Complex Questions over Knowledge Bases

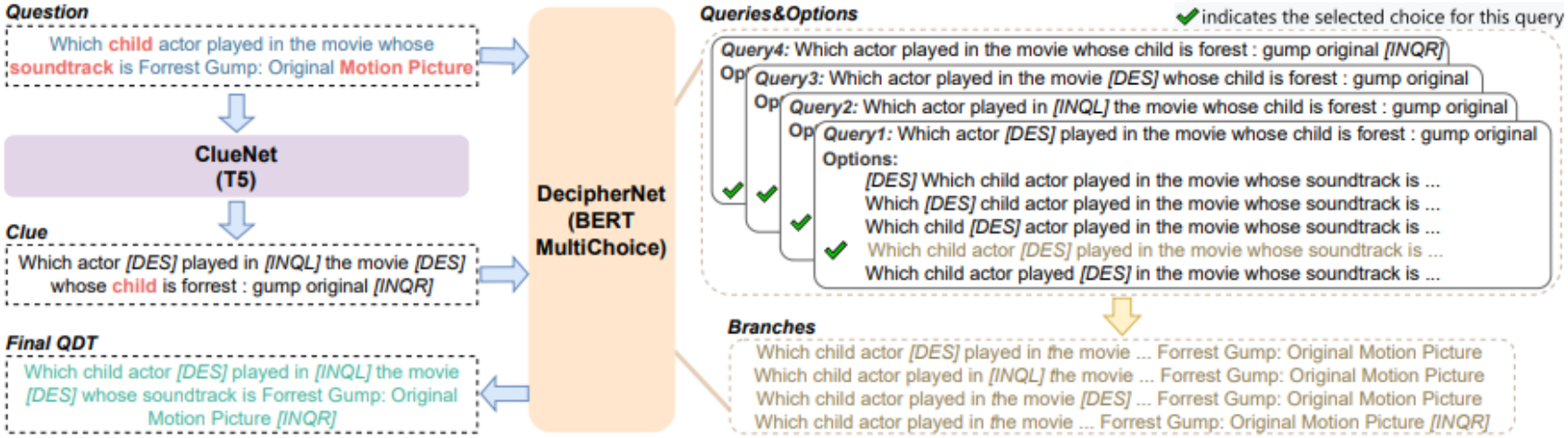
Question Decomposition Tree (QDT)

- Complex Questions
  - Assumption: can be decomposed into some simple questions
- Previous methods split a question into only two-parts
  - Insufficient to represent complex reasoning structure
- Tree-based decomposition
  - Recursively defined
  - Better decomposition structure
  - Can be Linearized to a sequence
    - Introducing some tags for generation



Decomposition Method (Clue-decipher)

- Mitigation of hallucination by tag insertion
- two-staged method
  - 1. generate the decomposition (using the generation ability)
  - 2. adopt a multi-choice model to determine inserting position for each tag (mitigating hallucination)



Experiments – Decomposition Results

- Compare with tree-based and sequence-based methods
  - Different metrics
- Annotate a dataset QDTrees from complex datasets and test on it
- Clue-decipher significantly outperforms other methods

Method	EM	TDA	GED
EDGQA (Hu et al. 2021)	-	0.7315	0.3799
`Clue-Decipher`	**0.8332**	**0.9650**	**0.0554**
w/o DecipherNet	0.8130	**0.9650**	0.0558

Table 3: Tree-based Decomposition evaluation.

Method	EM	BLEU	ROUGE
SplitQA (Talmor and Berant 2018)	0.653	0.734	0.905
DecompRC (Min et al. 2019)	0.862	0.954	0.988
HSP (Zhang et al. 2019)	0.252	0.679	0.881
HSP + DecipherNet	0.793	0.935	0.983
`Clue-Decipher`	**0.909**	**0.970**	**0.993**
w/o DecipherNet	0.889	0.966	0.991

Table 4: Sequence-based Decomposition evaluation.

Experiments - KBQA

- Adopt KBQA as downstream task to showcase the effectiveness of QDT
- Significantly improve the result for **two** QA systems in **two** KBs
  - Tree-structured decomposition substantially boosts the result

Method	Avg. F1	Acc
(Qin et al. 2021)	0.462	-
(Huang, Kim, and Zou 2021)	0.682	-
T5-11B + Revise (Das et al. 2021)	0.582	0.556
CBR-KBQA (Das et al. 2021)	0.700	0.671
QDTQA	**0.728**	**0.679**
w/o QDT	0.715	0.666
w/o tree-based structure	0.720	0.670
w/ SplitQA	0.716	0.669
w/ DecompoRC	0.716	0.669
w/ HSP	0.717	0.669
w/ EDGQA	0.714	0.665

Method	P	R	F1	ΔF1
NSQA	0.448	0.458	0.445	-
STaG-QA	**0.745***	0.548	0.536	-
(Liang et al. 2021)	0.511	0.593	0.549	-
EDGQA	0.505	0.560	0.531	0
w/ SplitQA	0.496	0.576	0.533	+0.002
w/ DecompRC	0.521	0.609	0.561	+0.030
w/ HSP	0.433	0.507	0.467	-0.064
w/ Clue-Decipher	0.548	**0.635**	**0.588**	**+0.056**

Limitations

- We just do surface form decomposition (strong assumption)
- Contemporary LLMs already do well in question understanding
- Linking can be more difficult
  - With golden linking results, LMs can do quite well in complex datasets (95% F1 on ComplexWebQuestions)
  - Structures can be well learned from annotations

- In Seq2Seq era, we augment information in input, where is the difficulty?
  - What can be further done for the community?

MarkQA: A large scale KBQA dataset with numerical reasoning

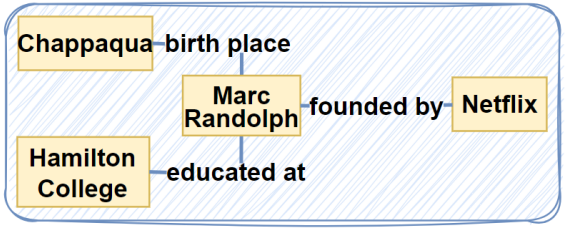
MarkQA: A large scale KBQA dataset with numerical reasoning

- KBQA aims to answer a question over a knowledge base (KB).
  - Need to match a **graph pattern** in the KB

- Numerical Reasoning is a critical ability in daily life
  - Require the ability of arithmetic, aggregation, comparison…

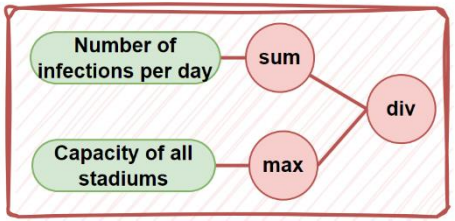
Multi-hop Reasnoing

Which company whose founder was born in Chappaqua and educated at Hamilton College?



Numerical Reasoning

How many of Japan's largest sports stadiums could be filled with the number of new COVID-19 infections in Japan in 2021?



MarkQA: A large scale KBQA dataset with numerical reasoning

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  - Need to match a **graph pattern** in the KB

- Numerical Reasoning is a critical ability in daily life
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Acquire some Information → **Further Process the Information**

Multi-hop Reasnoing

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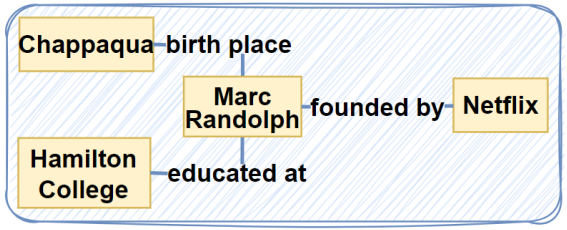

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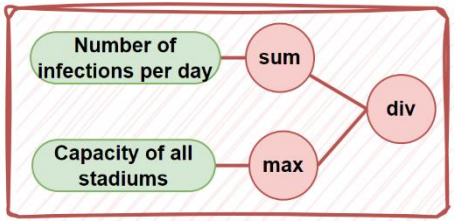
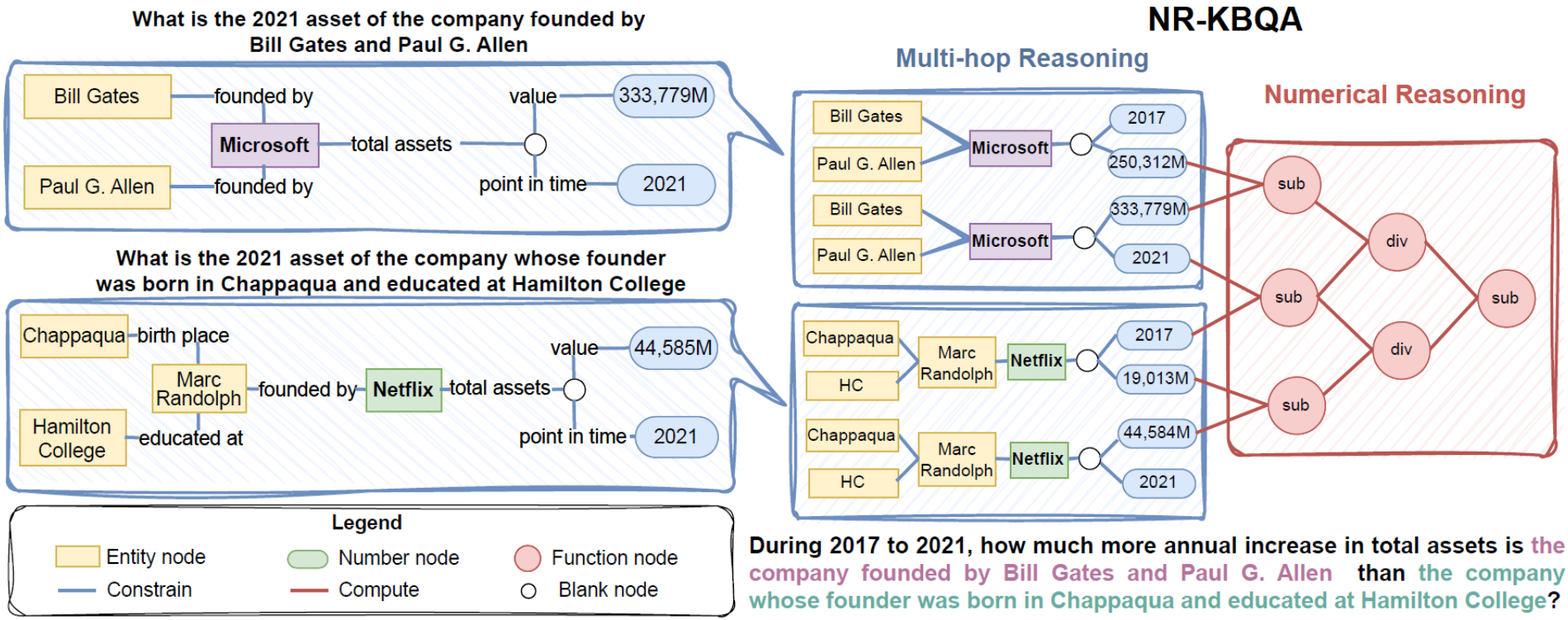


Motivation – previous datasets: few and simple

- Previous KBQA dataset mainly focus on Multi-hop reasoning(MR)
  - 90% of question in CWQ
  - 84.8% of question in GrailQA
- Numerical reasoning is insufficient in current KBQA datasets
  - Account for a small proportion
  - Only focus on Count, Argmax, Compare
  - Require calculation at most once
- For the first time explore and discuss Numerical Reasoning in KBQA from:
  - Task
  - Reasoning path representation
  - Dataset
  - Experiment

A New Task -- NR-KBQA



A New Representation -- PyQL

- Represented as a set of Python code
  - PyQL(Pythonic Query Language for SPARQL)
  - Each line initialize a PyQL object or calls a function

- Encapsulate various SPARQL syntax elements
  - BGP, Aggregation, Filter, Subquery, Assignment…
  - Can directly compiled to SPARQL

- Advantages:
  - User-friendly and conciseness
  - Step-by-Step reasoning path

PyQL

What is the average speed of all anti-aircraft gun with a range greater than 6,000 meters?

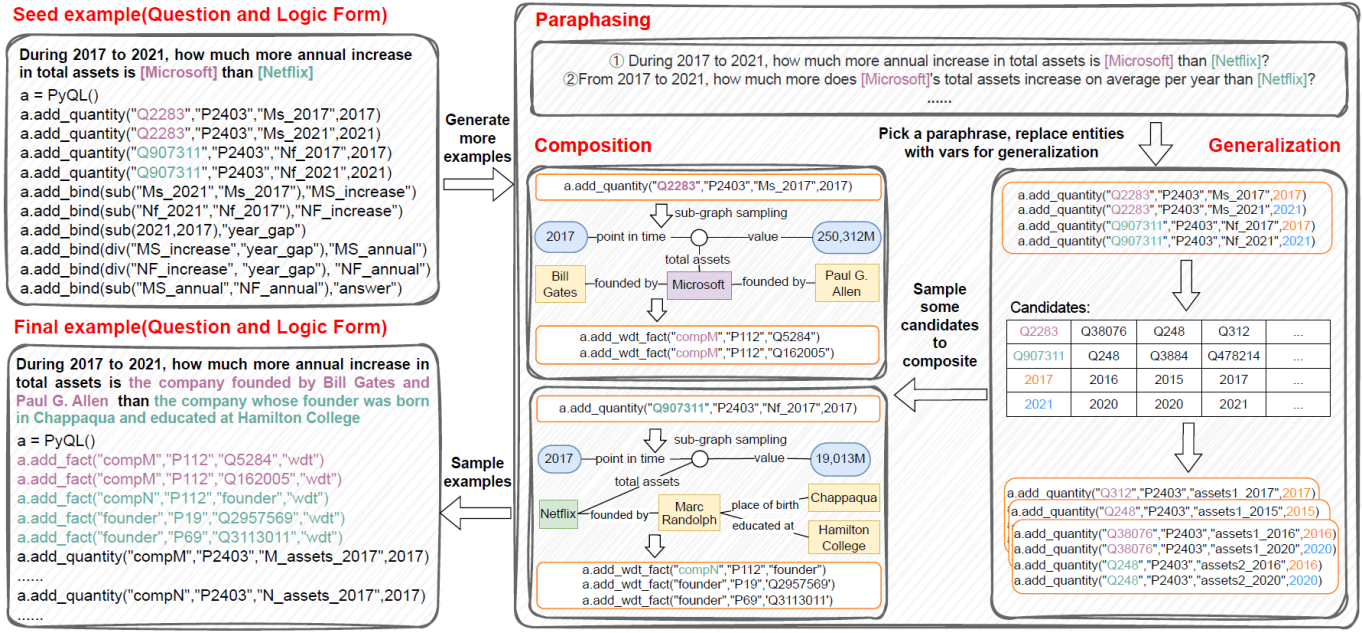
```
a=PyQL()
a.add_type_constrain('Q7325635','x1')
a.add_quantity('x1','P4176','x2')
a.add_filter('x2','>',6000)
a.add_quantity('x1','P2052','x3')
a.add_avg('x3','x4')
```

SPARQL

```
SELECT (AVG(?x3) AS ?x4 ) {
   ?x1 wdt:P31/wdt:P279* wd:Q7325635.
   ?x1 p:P4176 ?statement_x2.
   ?statement_x2 psv:P4176 ?value_st_x2.
   ?value_st_x2 wikibase:quantityAmount ?x2.
   FILTER(?x2 > 6000).
   ?x1 p:P2052 ?statement_x3.
   ?statement_x3 psv:P2052 ?value_st_x3.
   ?value_st_x3 wikibase:quantityAmount ?x3.
}
```

A New Dataset -- MarkQA

- Dataset Construction
  - Starts from 1K questions posed by humans and automatically scales to 32K examples. The construction framework: Seeds-to-Forest(SoF) consist of four steps:
    - Seeds Collection
    - Paraphrase
    - Generalization
    - Composition



Experiment

- Overall experiments

Methods	Output	Overall	I.I.D	Compositional	Zero-shot
T5-base	SPARQL	34.24	70.05	53.71	6.32
	PyQL	40.70	78.32	63.10	10.39
GMT	SPARQL	38.68	78.32	63.58	6.07
	PyQL	43.63	82.10	68.33	11.71
QDTQA	SPARQL	37.19	76.82	57.37	7.01
	PyQL	42.57	84.59	70.89	7.01

Table 2: QA performance (%) on test set of MarkQA.

Experiment

- Different reasoning type

Type	Over.	I.I.D	Comp.	Zero.
All	40.7	78.3	63.1	10.4
NR	42.0	85.4	64.3	12.9
NR and MR	38.5	65.5	61.8	5.1
NR and MR(1)	43.3	70.1	70.2	6.5
NR and MR(2)	28.7	55.6	44.8	2.3

Table 4: Performance of different types of questions on T5 (PyQL). NR and MR mean numerical reasoning and multi-hop reasoning, respectively. MR(1) and MR(2) mean one-hop and two-hop reasoning, respectively.

- Oracle experiment

Methods	Over.	I.I.D	Comp.	Zero.
T5-base	40.7	78.3	63.1	10.4
w/ gold E	46.5	88.3	72.7	12.1
w/ gold R	47.9	79.2	65.5	23.1
w/ gold ER	57.6	89.8	76.1	31.9

Table 3: Detailed analysis of T5-base with PyQL as output. w/ gold E or R means we use golden entity or relation linking results. Over., Comp., and Zero. stands for Overall, Compositional, and Zero-shot, respectively.

Limitations

- A lot human labor is involved in annotation
- PyQL query can be generalized to other environments

- How to well leverage PyQL query?
  - We prove the difficulty brought by structure, but how to handle it?
- How to incorporate LLMs?
  - LLMs can well handle question understanding, but how to introduce the schema?
  - Maybe by **interaction**, but how to design the interplay between input and output?

Running time, query engine times, LLM token cost

QueryAgent: A Reliable and Efficient Reasoning Framework with Environmental Feedback based Self-Correction

An LLM-based agent framework
for query building

Motivations

- PyQL query is step-wise-executable → step-by-step query building
  - An interface with knowledge base (retrieval tools and functional tools)
- End2End ICL generation with LLMs induce massive enumeration and hallucination
  - Can adopt question decomposition for better understanding and use LLMs reasoning ability
- Agent-based methods suffer from error propagation and hallucination
  - A novel correction method for reliable generation

PyQL

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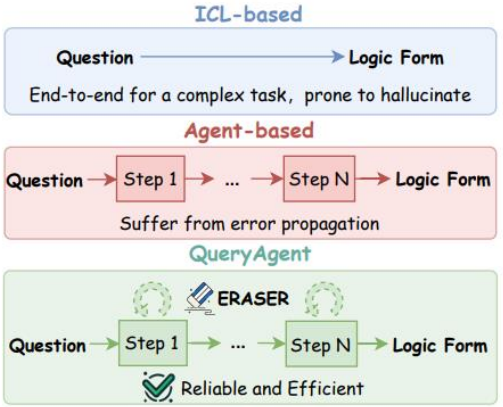
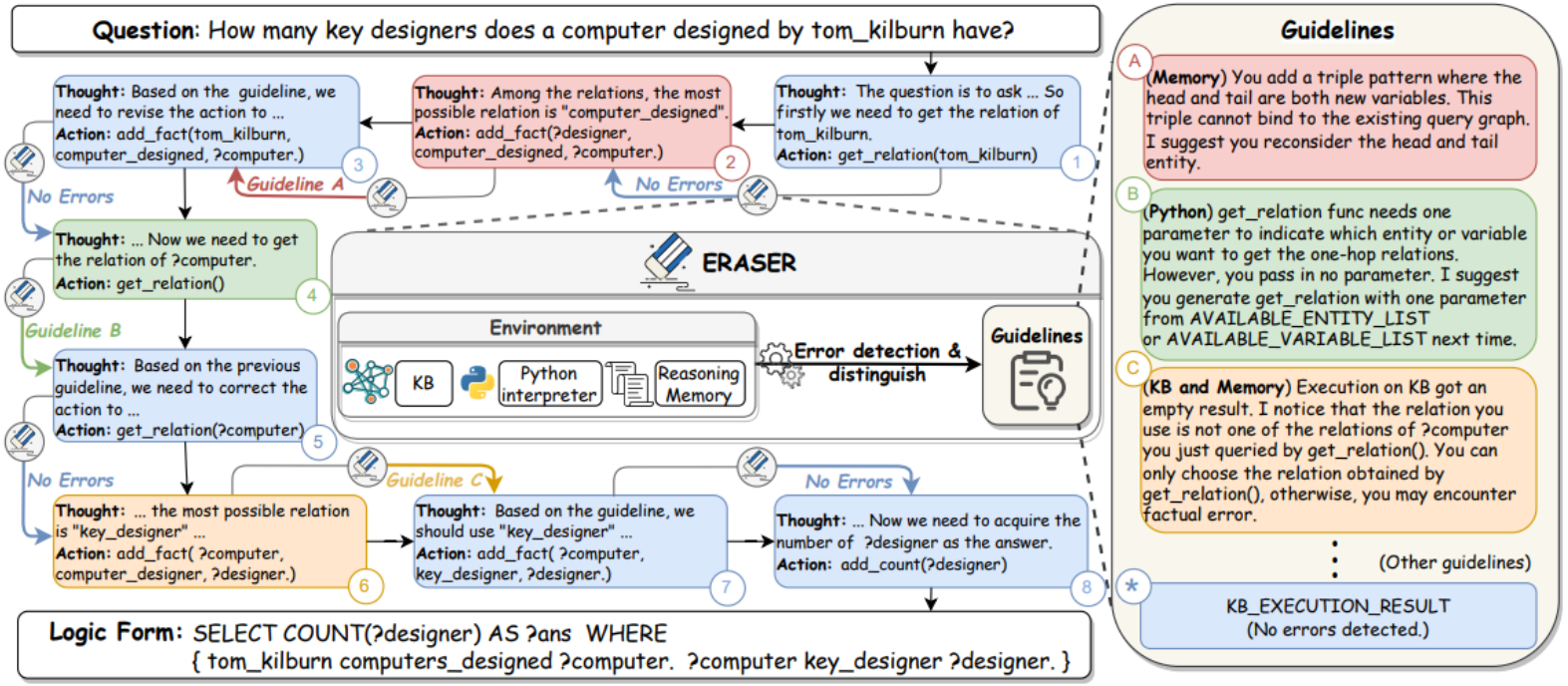


Figure 1: QueryAgent compared with two mainstream KBQA paradigms employing LLMs.

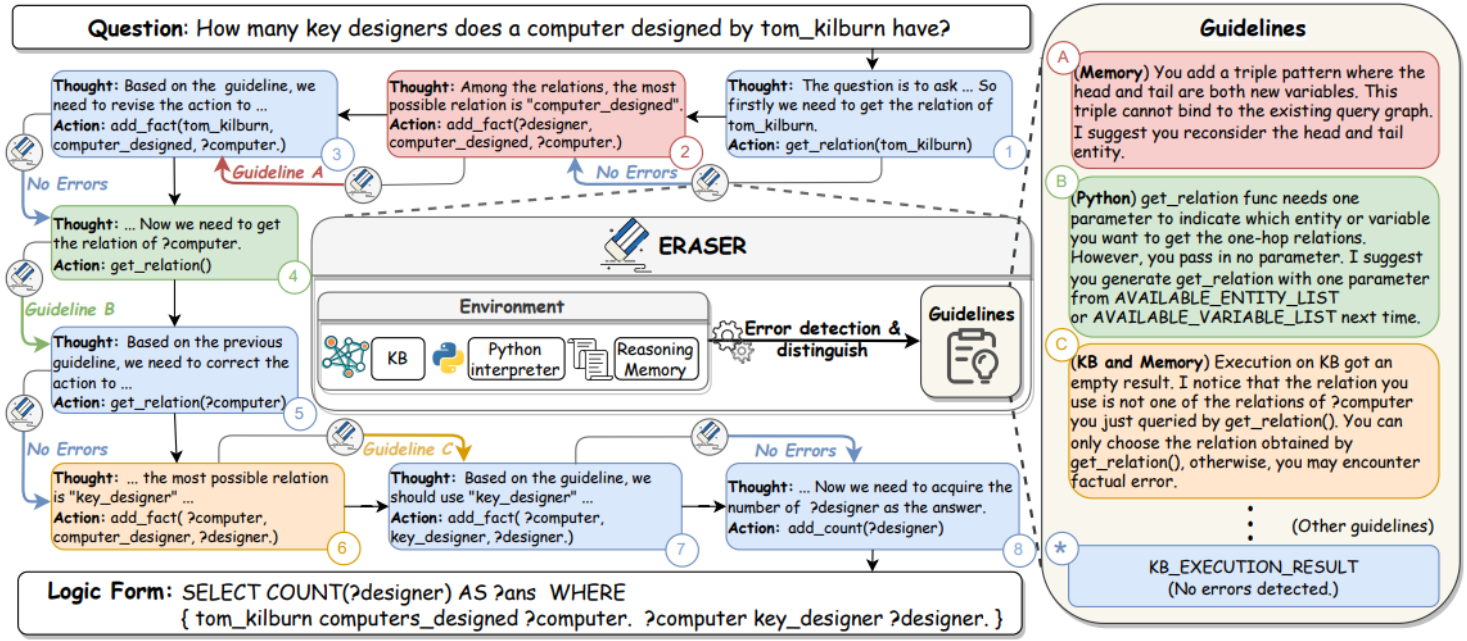
Agent framework (ReAct) with feedback-based self-correction

- Agent framework – step-by-step query building with PyQL function tools
  - based on previous step, an LLM generates thought and action. The action is executed. A correction module, ERASER, detects and distinguishes possible error and collect guidelines and add it to observations.



ERASER

- provide guidelines for possible hallucination
  - Previous: few-shot correction, relying on LLMs to identify the error and mimic the examples
  - Multiple feedback sources: KB engine, python interpreter and reasoning memory
  - Provide guidelines as observation (zero-shot, seamless correction)



Experiments

- Significant improvement with only one-shot example

Methods	GrailQA	GraphQ	WebQSP	MetaQA-3Hop
fine-tuning				
ArcaneQA (Gu and Su, 2022)	73.7	31.8	75.6	-
TIARA (Shu et al., 2022)	78.5	-	76.7	-
DecAF (Yu et al., 2023)	81.4	-	78.8	-
Pangu(T5-3B) (Gu et al., 2023)	83.4	57.7	79.6	-
few-shot				
Pangu (Gu et al., 2023)	53.5	35.4	48.6	-
KB-BINDER (Li et al., 2023)	50.8	34.5	56.6	96.5
KB-Coder (Nie et al., 2023)	51.7	35.8	60.5	-
one-shot				
KB-BINDER (Li et al., 2023)	16.8	4.8	9.0	65.3
AgentBench (Liu et al., 2024)	30.5	25.1	26.4	-
Ours	**60.5**	**50.8**	**63.9**	**98.5**
w/ GPT4	66.8	63.0	69.0	99.9

Analysis

- Ablation study of ERASER
- Transferability of ERASER
- Efficiency in runtime, engine query time and token cost

Method	GrailQA	GraphQ
Ours	**60.5**	**50.8**
w/o ERASER	43.7	35.3
w/ zero-shot SC	38.5	30.2
w/ few-shot SC	48.0	40.1

Ablation study

Methods	GrailQA	GraphQ	WebQSP
AgentBench	30.5	25.1	26.4
w ERASER	**38.5**	**35.6**	**32.0**

Transferability

Methods	GrailQA			GraphQ			WebQSP		
	TPQ	QPQ	CPQ	TPQ	QPQ	CPQ	TPQ	QPQ	CPQ
KB-BINDER	51.2 s	3297.7	**$ 0.010**	84.0 s	2113.8	$ 0.024	138.6 s	8145.1	$ 0.017
AgentBench	40.0 s	7.4	$ 0.034	65.1 s	7.2	$ 0.035	70.4 s	7.2	$ 0.038
Ours	**16.6 s**	**5.2**	$0.019	**15.3 s**	**6.2**	**$ 0.021**	**12.6 s**	**4.7**	**$ 0.014**

Efficiency analysis

Limitations

- The correction guidelines are well crafted and based on diverse feedback
  - Based on the step-by-step manner, we have various feedback sources
- The step-by-step reasoning is a fine-grained decomposition
  - Lead to lengthy prompts
  - We LLMs understand a complex question well. Maybe we can achieve a different way of interaction
  - (human and animals tend to have a plan substantially and ground the plan in environments.)

1. Idioms (when sharing business cards)
2. Call LLMs (how to practically invoke LLMs)

Call me when necessary:
LLMs can Efficiently and Faithfully Reason over Structured Environments

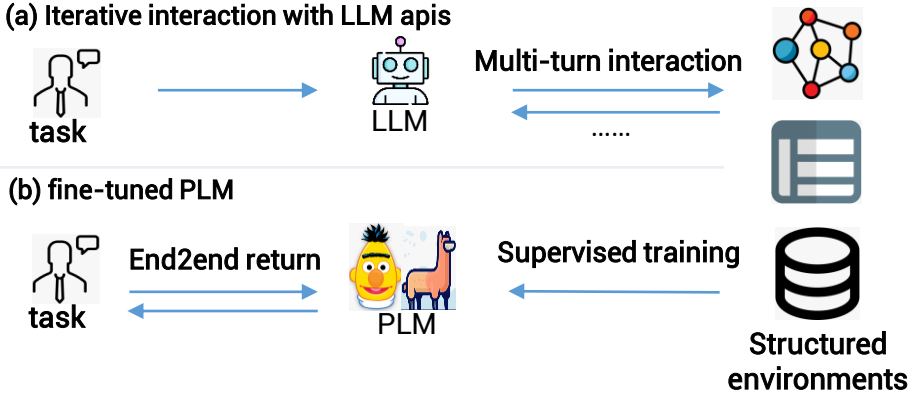
Less LLM calls

LLM's output can be grounded on environments

Multi-hop reasoning over Structured Environments (KG, Tables)

Previous interaction paradigms

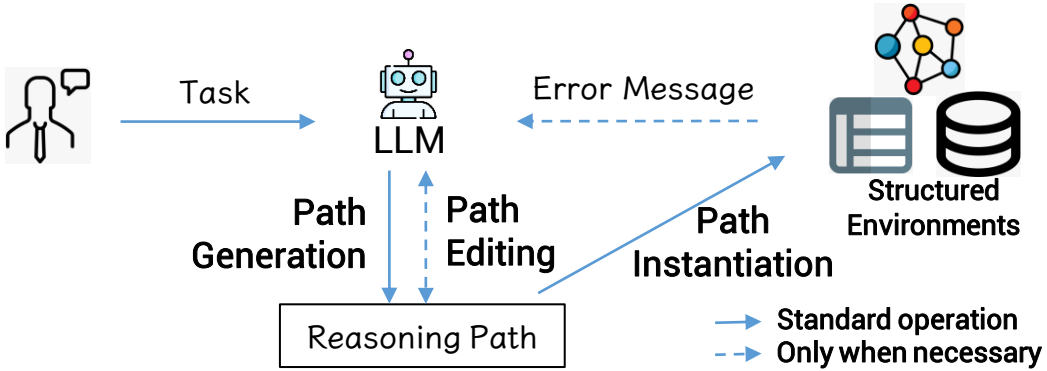
- Interactive interaction
  - minimum effort at each step
  - E.g.: Who is Obama's daughter?
    - Direct： Obama -> daughter
    - Iterative
      - » 1. relations around Obama
      - » 2. choose daughter
  - pros
    - Decomposition for smaller environmental space
    - LLM discriminate at each step (better faithfulness)
  - cons
    - Incremental and minimum effort can by inefficient
    - Each step rely on previous steps, inducing error propagation
    - Multi-hop question may introduce multiple steps and some entity may involve massive relations, introducing long history



- Injecting environments into models when training, End2End return when inference
  - Direct path generation or Retrieval-and-Build
  - Pros: no interaction at inference time, better efficiency
  - Cons:
    - Not ensuring faithfulness and relying on beam search, resulting in larger retrieved instances
    - Relying heavily on training data, hard to obtain for large-scale environments

Reasoning Path Editing (Readi)

- How humans interact？ How do we do multi-hop reasoning?
  - Which college did Obama's daughter go to? Obama → daughter → college …
- "Reasoning path" to represent structured reasoning process
  - Utilize strong understanding ability of LLMs
  - Can be instantiated on environments, bridging the heterogeneity gap
- LLMs interacting framework to build a reasoning path
  - End-2-end generation of an initial reasoning path (less LLM calls)
  - Instantiation on environments， edit the path when anything goes wrong (better faithfulness)



Reasoning path

- Structured representation of natural language task
  - Instantiable on structured environments (Knowledge graph)
- Relational path from topic entities
- Can represent complex constrains (conjunction)

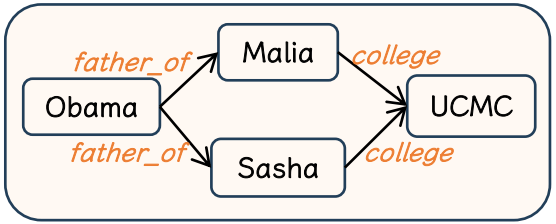
Example $Q1$

Where did daughters of Obama go to college?

Reasoning Path

[Obama] father_of→college

Path Instances



Single-constrained Reasoning Path

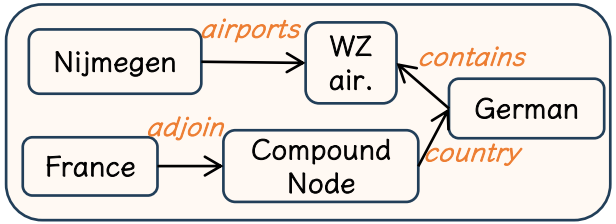
Example $Q2$

What country bordering France contains an airport that serves Nijmegen?

Reasoning Path

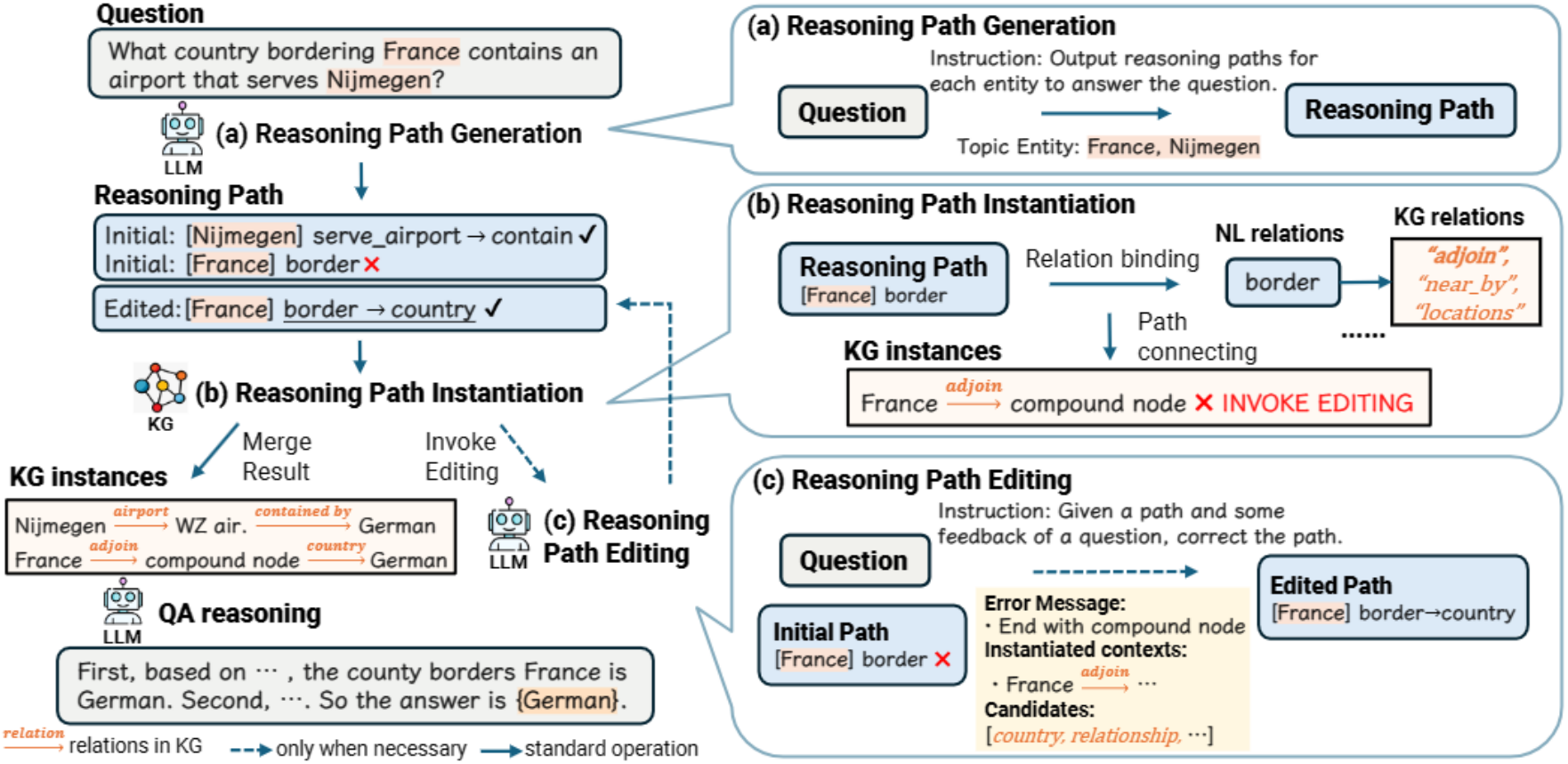
[Nijmegen] serve_airport→contain
[France] border→country

Path Instances



Multi-constrained Reasoning Path

Method – Reasoning Path Editing (Readi)



Method – Reasoning Path Editing (Readi)

- End-to-End initial path generation (based on in context learning)
  - What country bordering France contains an airport that serves Nijmegen?
    - [Nijmegen] serve_airport→contain
    - [France] border→country

Prompts for reasoning path generation

Given a question and some Topic Entities in the Question, output possible freebase Relation Paths starting from each Topic Entities in order to answer the question.

Demonstration Example

Question: Find the person who said "Taste cannot be controlled by law", where did this person die from?

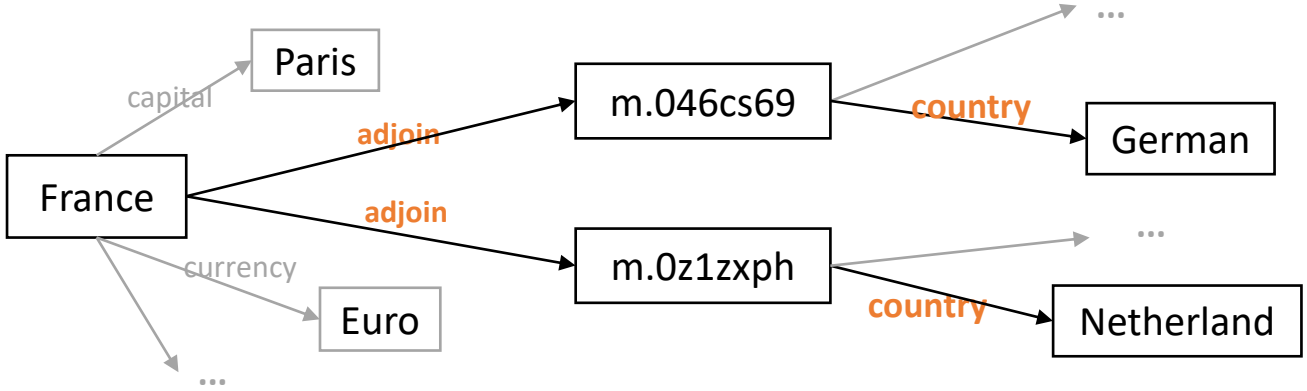
Topic Entities: ["Taste cannot be controlled by law"]

Thought: There is only one topic entity, the answer is constrained by one path. For, the path from "Taste cannot be controlled by law", firstly, it should cover the person quote it. Second, it should cover the place where the person died.

Path: { "Taste cannot be controlled by law": [Taste cannot be controlled by law → people.person.quotations → people.deceased_person.place_of_death]}

Method – Reasoning Path Editing (Readi)

- Reasoning path instantiation:
  - First bind NL relations to knowledge base relations, then connect the relations (BFS)
    - Reasoning path: [France] border → country
    - Relation binding:
      - **border :** {adjoin, near_by, locations}
      - **country :** {country, locations, county}
    - Path connecting: France – adjoin – cvt node – country - ...



cvt node: compound value node in Knowledge graphs

Method – Reasoning Path Editing (Readi)

- Collect error messages for LLMs to edit previous path
  - Error reasons: cvt ending, empty reasoning path, current relation cannot be connected
  - Error messages: error reasons, instantiation progress, candidate relations

Prompts for reasoning path editing

Task: Given an Inital Path and some feedback information of a Question, please correct the initial path.

Demonstration Example

Question: The movie featured Miley Cyrus and was produced by Tobin Armbrust?

Initial Path: Miley Cyrus→film.film.actor→film.film.producer Error Message

1. <compound node> in the end.

2. relation "film.film.producer" not instantiated.

Instantiation Context

Instantiate Paths: Miley Cyrus → film.actor.film → <compound node>

Candidate Relations

['film.director.film', 'film.performance.film', ...]

Corrected Path

Goal: The Initial Path starts from Miley Cyrus, which should cover the movies featured by Miley Cyrus.

Thought: In Instantiate Paths I know that Miley Cyrus acts some films, described by a compound node. In candidates, I find "film.performance.film" most relevant to get the films. Meanwhile, "film.film.producer" is not relevant to my Goal.

Final Path: Miley Cyrus→film.actor.film→ film.performance.film

Experiments – Main Results

Methods	WebQSP	CWQ	MQA-1H	MQA-2H	MQA-3H
Training-based Method					
EmbedKGQA (Saxena et al., 2020)	66.6	-	**97.5**	98.8	94.8
NSM (He et al., 2021)	67.7	47.6	97.1	99.9	98.9
TransferNet (Shi et al., 2021)	71.4	48.6	97.5	**100***	**100***
SR+NSM+E2E (Zhang et al., 2022)	69.5	49.3	-	-	-
UniKGQA (Jiang et al., 2023c)	75.1	50.7	**97.5**	99.0	99.1
ReasoningLM (Jiang et al., 2023b)	78.5	**69.0***	96.5	98.3	92.7
RoG (Luo et al., 2023)	**85.7***	62.6	-	-	84.8
Inference-based Method					
Davinci-003 (Ouyang et al., 2022)	48.7	-	52.1	25.3	42.5
GPT3.5 (OpenAI, 2022)	65.7	44.7	61.9	31.0	43.2
GPT4 (OpenAI, 2023)	70.7	52.1	71.8	52.5	49.2
AgentBench (Liu et al., 2023b)	47.8	24.8	-	-	-
StructGPT (Jiang et al., 2023a)	69.6	-	97.1	97.3	87.0
Readi-GPT3.5	74.3	55.6	98.4	**99.9**	**99.4**
Readi-GPT4	**78.7**	**67.0**	**98.5***	**99.9**	99.2

KBQA （Hit@1）

Methods	WTQ	WikiSQL
Training-based Method		
TAPAS	48.8	83.6
UnifiedSKG (T5-3B)	49.3	86.0
TAPEX	**57.5**	**89.5**
Inference-based Method		
Davinci-003	34.8	49.1
GPT3.5	55.8	59.8
GPT4	57.0	59.9
StructGPT	52.2	65.6
Readi-GPT3.5	**61.7**	**66.2**
Readi-GPT4	61.3	66.0

TableQA （denotation accuracy）

Analysis - Ablation Study (generation and editing modules)

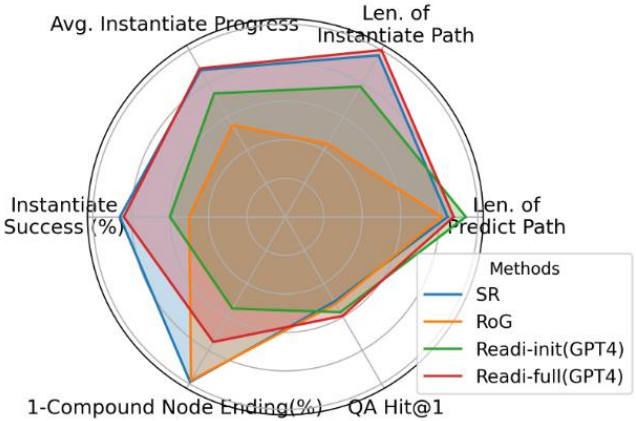
- Effectiveness of initial path generation (horizontal)
- Effectiveness of path editing (vertical)
  - Editing for corrupt and empty path shows robustness
- From left to right, from top to bottom, all show an upward trend
  - With stronger model, comes better results
- Plug-and-play nature for initial path generation and editing

Variance of Readi	Answer Coverage Rate (AC)				QA Performance (Hit@1)			
	Corrupt	*Empty*	GPT3.5	GPT4	*Corrupt*	*Empty*	GPT3.5	GPT4
w/o edit	-	-	56.7	62.7	-	-	51.0	57.2
w/ edit by GPT3.5	54.0	56.4	62.5	64.3	57.3	58.5	58.7	58.5
w/ edit by GPT4	55.6	63.9	68.6	65.8	58.2	59.9	58.1	59.3

Analysis – Features of reasoning path

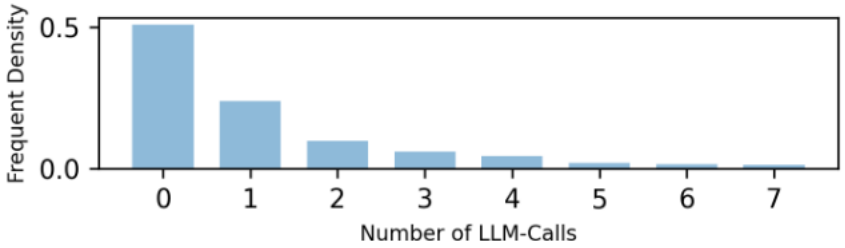
- Readi's initial path is competitive
  - GPT3.5 initial reasoning path is on par the finetuned methods
  - GPT4 initial reasoning path better than finetuned methods
- After editing, Readi's path outperforms finetuned methods with wider beams
- Finetuned methods get exploded number of retrieved knowledge with wider beams
  - Still worse QA results than Readi

Methods	Graph Quality		QA Perf.
	AC	#RK	Hit@1
SR			
- beam size 1	58.4	**26.3**	50.9
- beam size 3	67.2	47.1	54.6
RoG			
- beam size 1	57.0	69.5	52.2
- beam size 3	**77.5**	170.1	57.3
Readi initial path			
- GPT3.5	56.7	134.6	51.0
- GPT4	62.7	101.4	57.2
Readi full			
- GPT3.5	62.5	93.7	58.7
- GPT4	71.8	121.5	**59.3**



Analysis - Efficiency

- Distribution of LLMs editing times
  - Averagely 1.55 – GPT4, 1.99 – GPT3.5
  - Half questions does not need editing (LLM called only once)



Limitations

- Can try other LLMs to test generalizability of our framework
- The Instantiation is natural but a bit brute force
- The interaction is relatively efficient and faithful, does not ensure the instances we obtain can be used to answer the question
  - We adopt LLMs ability to generate reasoning path, the path can be fully instantiated does not mean the path is the ground truth
  - This is also the limitation of IR

Thanks for listening

- Q&A