



Language Models and Structured Knowledge in AI

12.09.2024

Dr. Gerrit Großmann, Islam Mesabah

github.com/gerritgr/LLMSummerSchool



dfki
ai
Deutsches Forschungszentrum
für Künstliche Intelligenz
German Research Center for
Artificial Intelligence

What to expect

Theory (30 min)



General introduction into multiple ideas



Details of every neuro-symbolic LLM concept, LLM agents, prompt engineering

Hands-on (2 hours)



Implementation of a KG-based RAG system based on Mistral and neo4j



Revising every software library for combining LLMs with structured knowledge

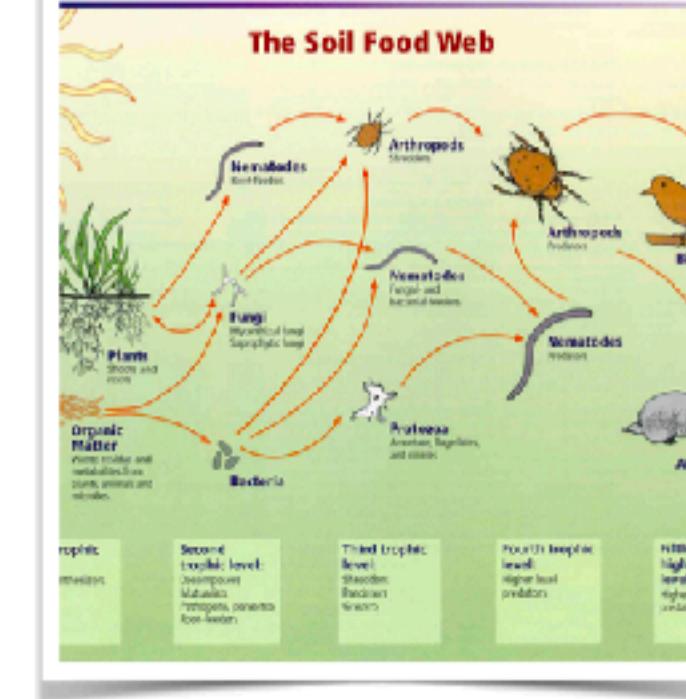
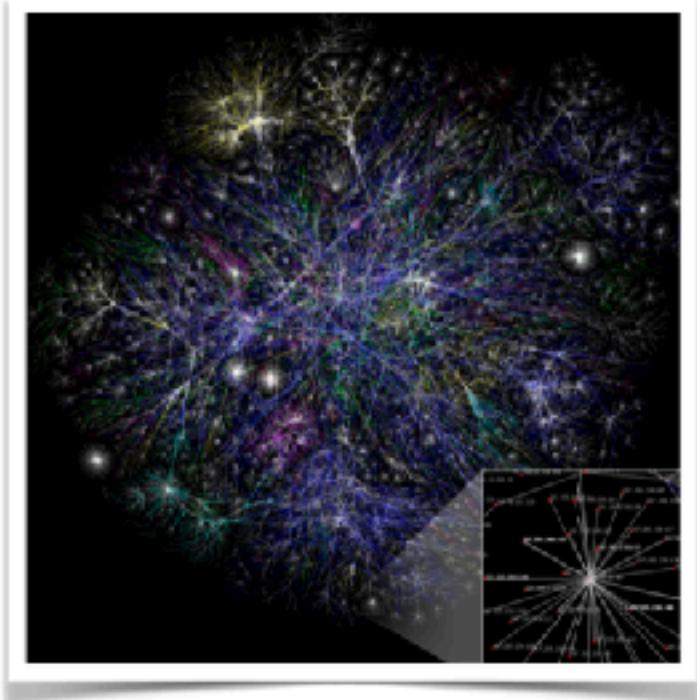
You know this.

Language Models and Structured Knowledge in AI

... not so obvious.

- Databases & tabular data
- XML and JSON files
- Programm code & rule-based models
- Knowledge graphs
- Labeled files

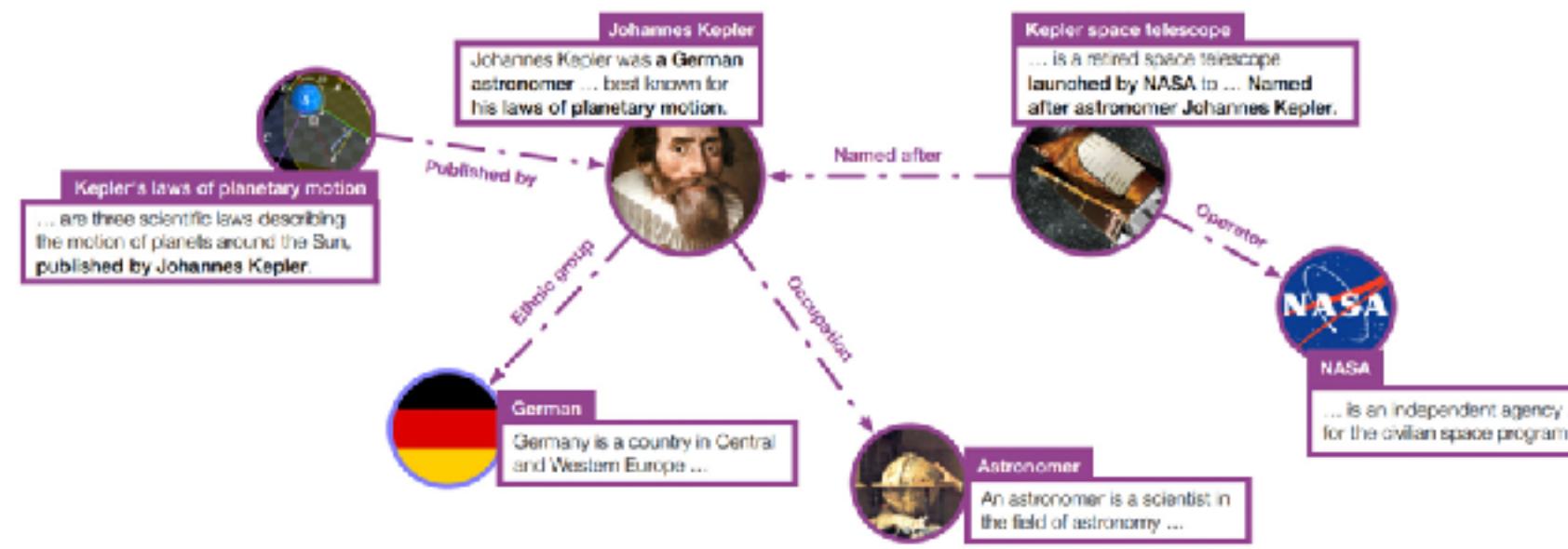
Why Graphs?



In many ways, graphs are the main modality of data we receive from nature.

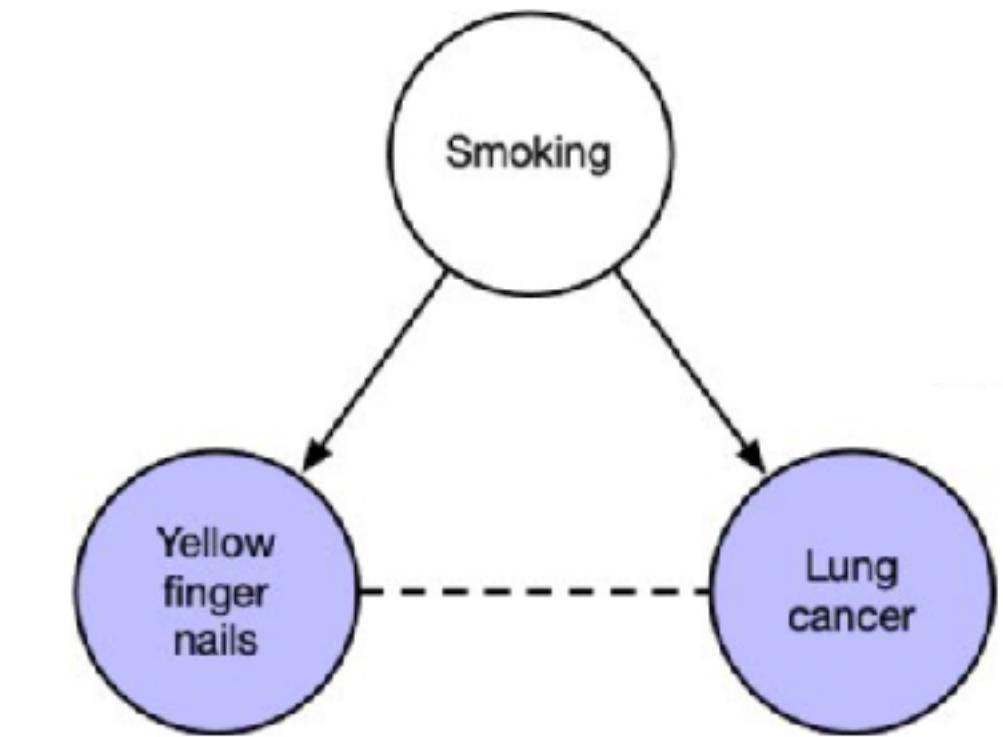
- Petar Veličković

Why Graphs?



<https://deepgraphlearning.github.io/project/wikidata5m>

Knowledge Graph



An introduction to causal reasoning in health analytics (Zhang et al)

Causal Graph



<https://towardsdatascience.com/visualizing-protein-networks-in-python-58a9b51be9d5>

Interaction Graph

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Why Graphs?



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Knowledge Graph

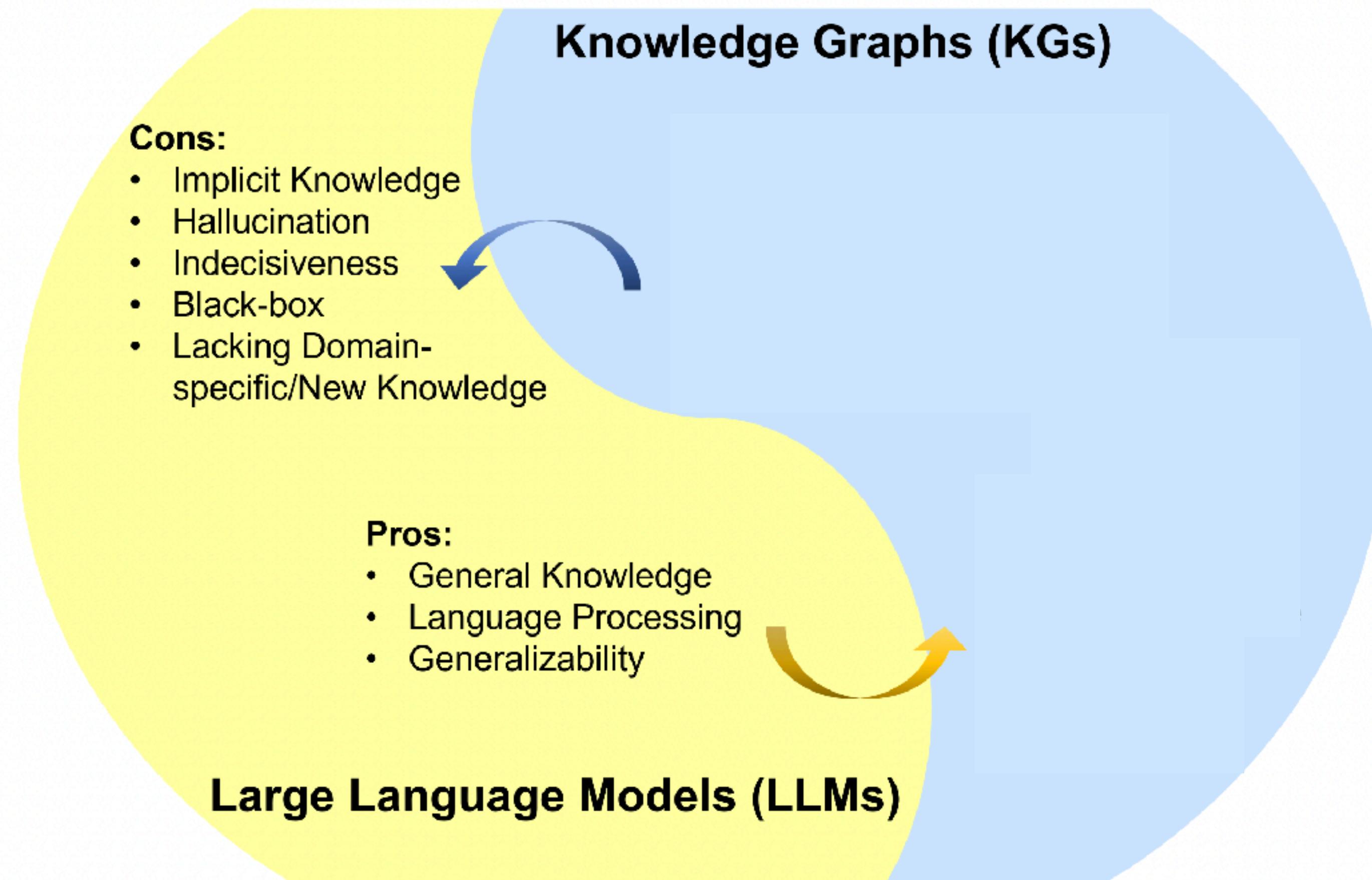
Causal Graph

Interaction Graph

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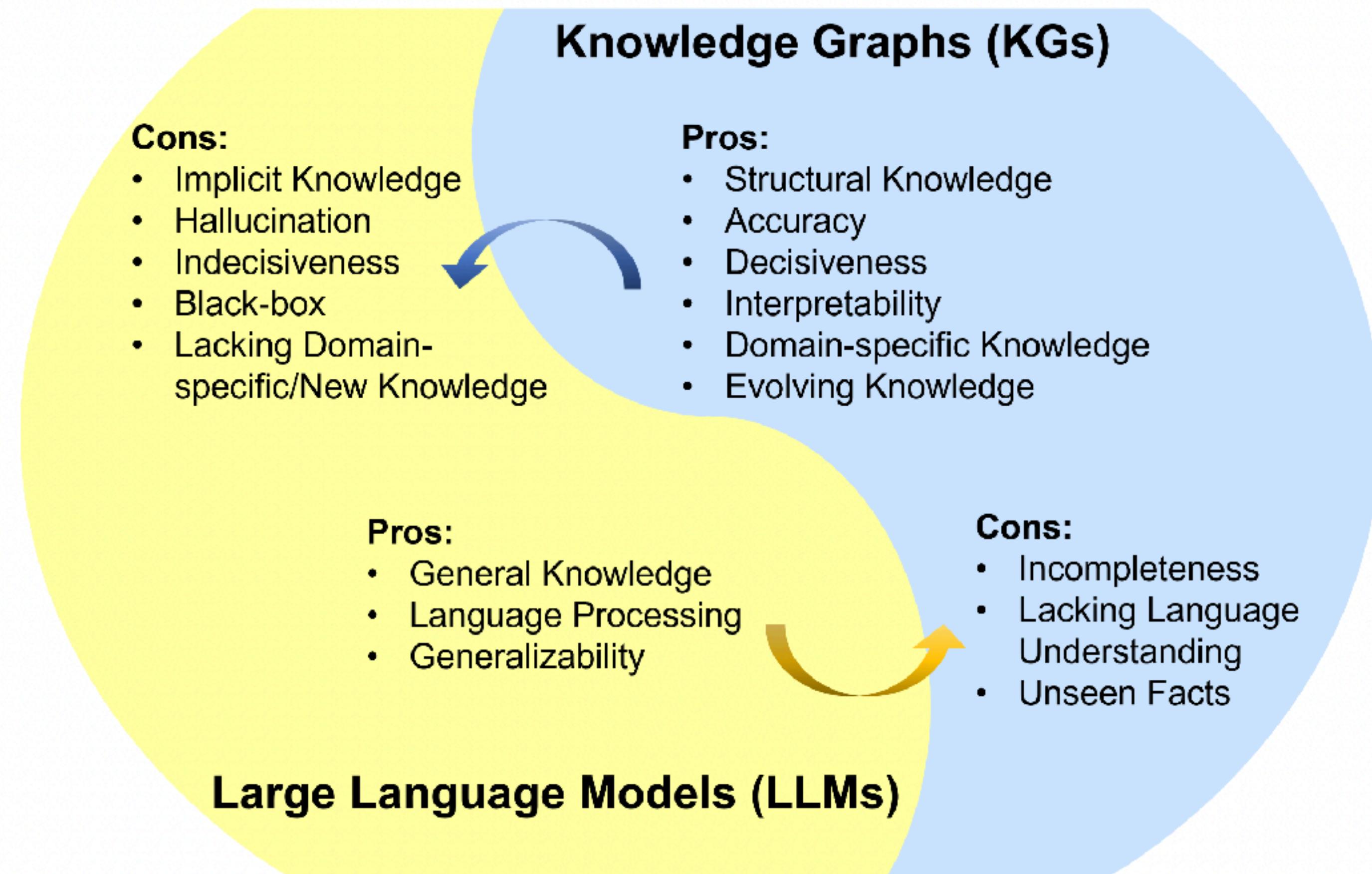
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Graphs and LLMs



Unifying Large Language Models and Knowledge Graphs: A Roadmap (Pan et al.)

Graphs and LLMs



Unifying Large Language Models and Knowledge Graphs: A Roadmap (Pan et al.)

Thriving Research

1. arXiv:2408.16667 [pdf, other] cs.LG cs.NI cs.CL cs.MA

Iterative Graph Alignment

Authors: Fangyuan Yu, Hardeep Singh Arora, Matt Johnson

Abstract: By compressing diverse narratives, LLMs go beyond memorization, achieving intelligence by capturing generalizable causal relationships. However, they suffer from local 'representation gaps' due to insufficient training data diversity, limiting their real-world utility, especially in tasks requiring strict alignment to rules. Traditional alignment met...

Submitted 29 August, 2024; originally announced August 2024.

Comments: 12 pages, 4 figures

2. arXiv:2407.13989 [pdf, other] cs.LG cs.AI

Enhancing Data-Limited Graph Neural Networks by Actively Distilling Knowledge from Large Language Models

Authors: Quan Li, Tianxiang Zhao, Lingwei Chen, Junjie Xu, Suhang Wang

Abstract: Graphs are pervasive in the real-world, such as social network analysis, bioinformatics, and...

Submitted 28 August, 2024; v1 submitted 18 July, 2024; originally announced July 2024.

Comments: 10 pages, 3 figures

3. arXiv:2408.15903 [pdf, other] cs.CL

LLM-Based Multi-Hop Question Answering with Knowledge Graph Integration in Evolving Environments

Authors: Ruirui Chen, Weifeng Jiang, Chengwei Qin, Ishaan Singh Rawal, Cheston Tan, Dongkyu Choi, Bo Xiang, Bo Ai

Abstract: The rapid obsolescence of information in Large Language Models (LLMs) has driven the development of various techniques to incorporate new facts. However, existing methods for...

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AnomalyLLM: Few-shot Anomaly Edge Detection for Dynamic Graphs using Large Language Models

Authors: Shuo Liu, Di Yao, Lanting Fang, Zhetao Li, Wenbin Li, Kaiyu Feng, Xiaowen Ji, Jingping Bi

Abstract: Detecting anomaly edges for dynamic graphs aims to identify edges significantly deviating from the normal pattern and can be applied in various domains, such as cybersecurity, financial transactions and AIOps. With the evolving of time, the types of anomaly edges are emerging and the labeled anomaly samples are few for each type. Current methods are either d...

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Comments: 13 pages

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WeKnow-RAG: An Adaptive Approach for Retrieval-Augmented Generation Integrating Web Search and Knowledge Graphs

Authors: Weijian Xie, Xuefeng Liang, Yuhui Liu, Kaihua Ni, Hong Cheng, Zetian Hu

Abstract: Large Language Models (LLMs) have greatly contributed to the development of adaptive intelligent agents and are positioned as an important way to achieve Artificial General Intelligence (AGI). However,...

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Comments: 8 pages, 2 figures, technical report for 3rd place in Task 3 of Meta KDD Cup 2024 CRAG Challenge

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Cross-Modal Learning for Chemistry Property Prediction: Large Language Models Meet Graph Machine Learning

Authors: Sakhinana Sagar Srinivas, Venkataramana Runkana

Abstract: ...is to create novel molecules with desired properties, facilitating accurate property predictions for applications such as material design and drug screening. However, existing graph deep learning methods face limitations that curb their expressive power. To address this, we explore the integration of vast molecular domain...

Submitted 27 August, 2024; originally announced August 2024.

Comments: Paper Accepted at Workshop on Deductive and Differentiable Reasoning in Generative Models at NeurIPS 2024

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Structured Data Analysis using Knowledge Graph + LLM

The post-2020 era is referred to as the digital era. Most companies are re-inventing their working model by digitizing...

Jan 20 · 259 · 3



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Ontotext Marketing Gets a Boost from Knowledge Graph Powered LLMs

An abbreviated and updated version of a presentation from Ontotext's Knowledge Graph Forum 2023 about the synergy...

Mar 13 · 14 · 1



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Build Product Knowledge Graph using LLM

Extracting attribute-value information from unstructured data is called named entity recognition. There are various ways of...

Aug 2 · 159 · 1



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Can you mention the tech stack to build knowledge graph based LLMs?

Nov 16, 2023 · 9 · 1



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Navigating the World of Knowledge Graphs : Part 1

Knowledge Graph with LLM Story

Nov 20, 2023 · 116 · 1



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It does now :) Take a look:

https://github.com/ahuinyk/knowledge_graph_maker/tree/main/knowledge_graph_maker/lm_clients

Jul 30



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Large language models(LLM) & Knowledge Graph(KG) : 1+1>2 ?

Erik Protocol has always been committed to building robust



Thriving Research

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Submitted 27 August, 2024; originally announced August 2024.

Comments: Detailed description of Workflows on GitHub and Preprint available in Generation Model at https://doi.org/10.5281/2



- New ideas every day
- Functioning ecosystem
- Easy to get started



- Impossible to keep track of everything

1. Materials
Structured Data Analysis using Knowledge Graph + LLM
The post-2020 era is referred to as the digital era. Most companies are re-inventing their working model by digitizing...
len 30 · 259 · 1 · ...

2. Ontext
Ontext Marketing Gets a Boost from Knowledge Graph Powered LLMs
An abbreviated and updated version of a presentation from Ontext's Knowledge Graph Forum 2023 about the synergy...
Aug 24 · 159 · 1 · ...

3. Prashant Dahiya - Towards AI
Build Product Knowledge Graph using LLM
Extracting attribute-value information from unstructured data is called named entity recognition. There are various ways of...
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4. E. Singh
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Nov 16, 2022 · 2 · ...

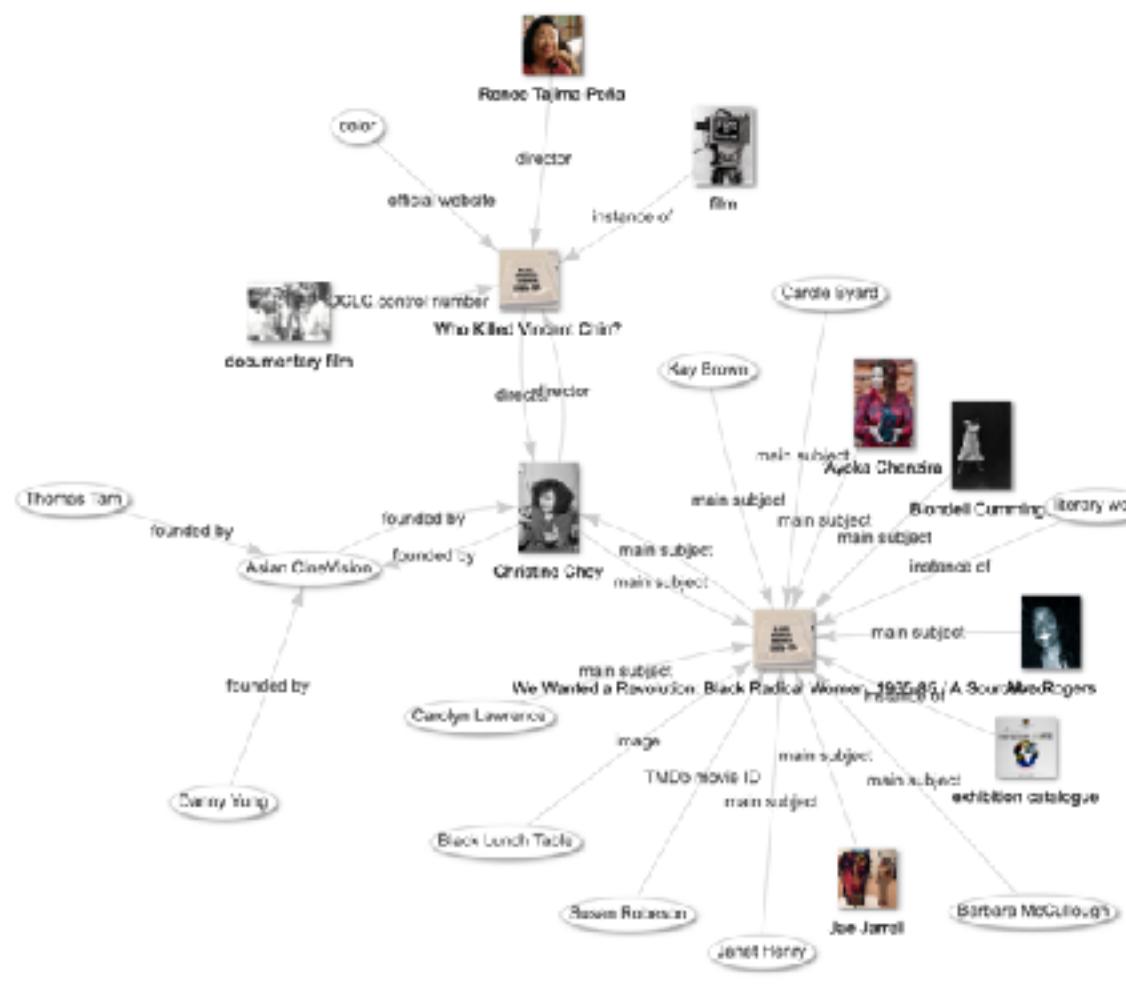
5. Adith Patel in ML Research Lab
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Nov 20, 2022 · 16 · ...

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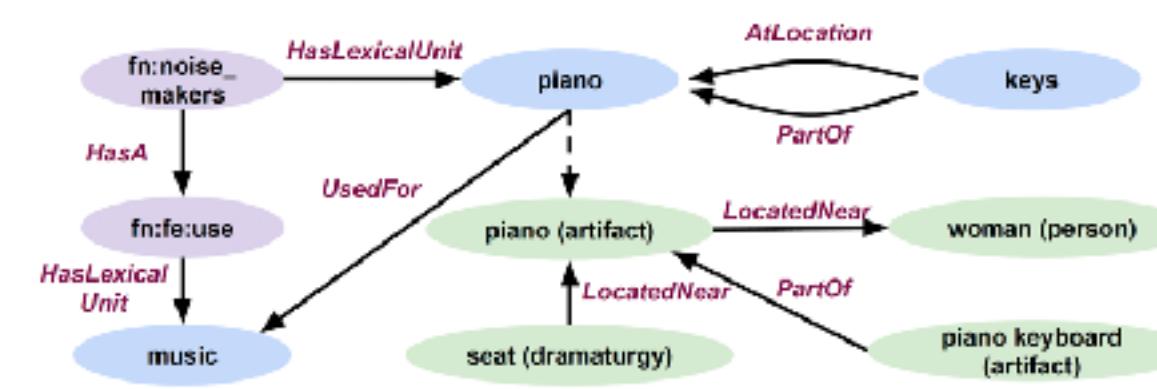
7. Edit Protocol
Large language models(LLM) & Knowledge Graph(KG) : 1+1>2 ?
Edit Protocol has always been committed to building robust...

What is a Knowledge Graph?

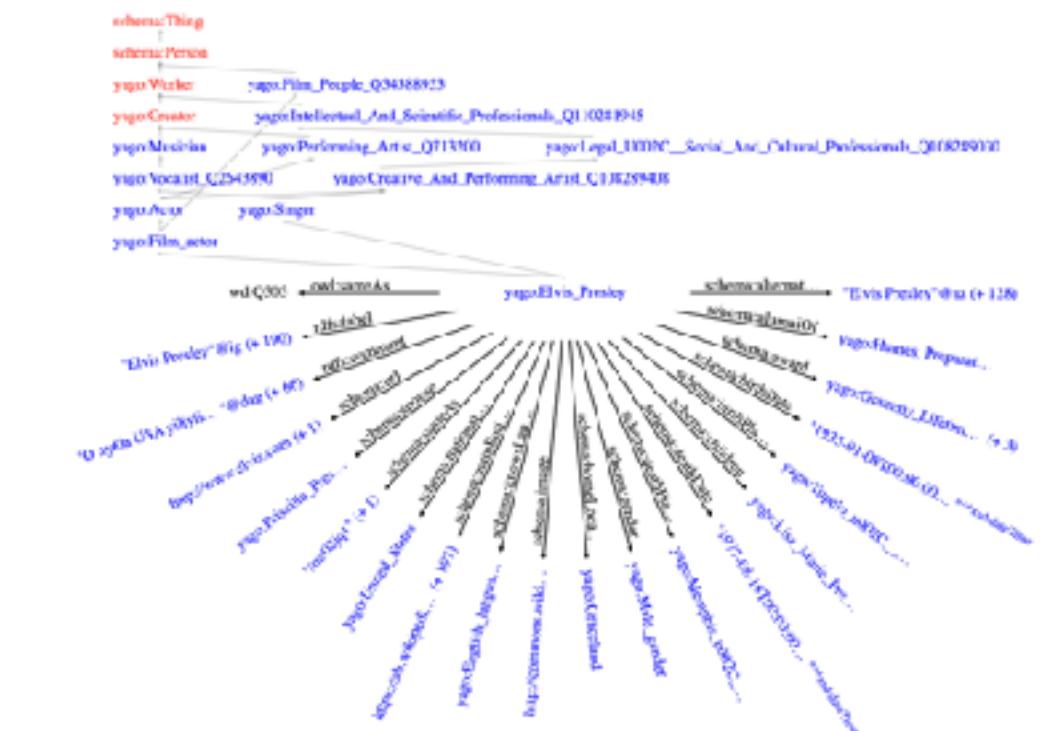
A KG consists of entities (**nodes**) that are connected by relationships (**edges**).
Typically represented as list of (**subject, predicate, object**) triplets



WikiData
> 100 million items



CSKG
> 2 million items



Yago
> 10 million items



DrugBank
20 thousand items

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Create private KG:



Financial Data



Medical data



Vacation Planning



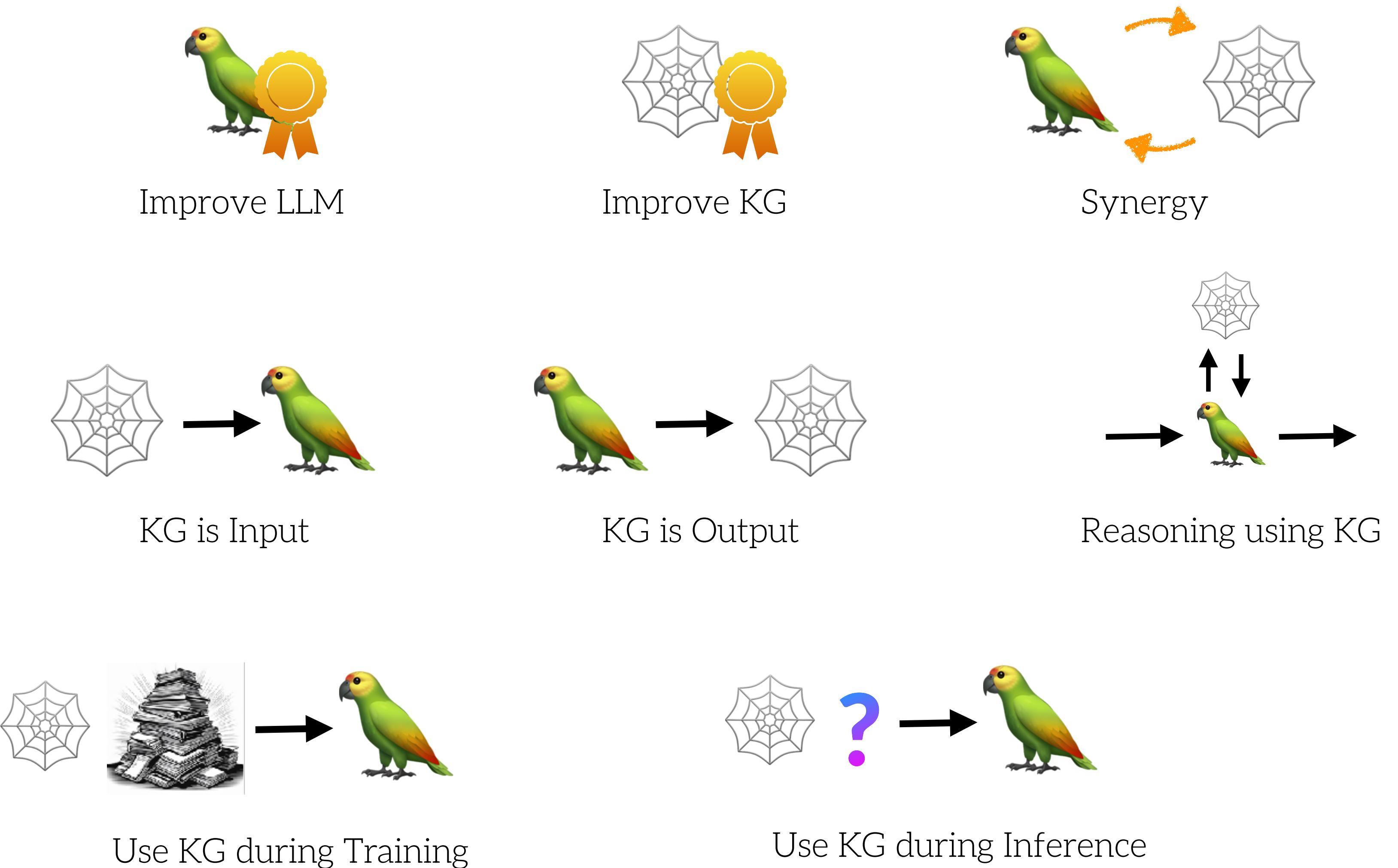
Reading List

Taxonomy

Goal

Input/Output

Training/Inference

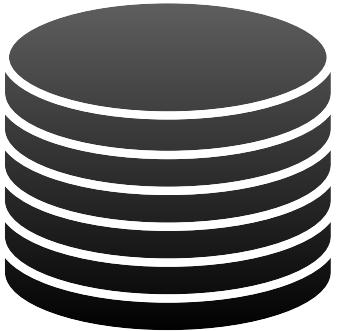




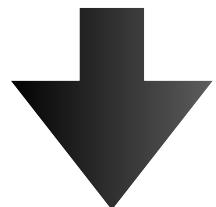
Part II

Some Great Ideas of KG and LLM Combinations

Constructing Graph Queries

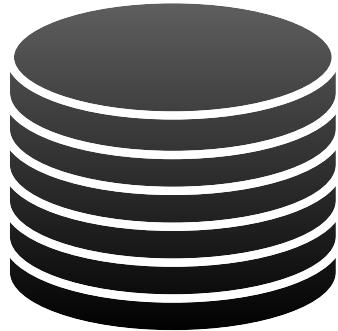


What are the names of the directors of all the movies Natalie Portman starred in between 2010 and 2020?

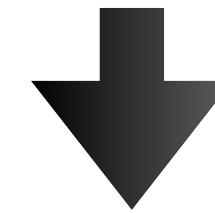


```
SELECT DISTINCT d.name AS director_name
FROM movies m
JOIN movie_cast mc ON m.movie_id = mc.movie_id
JOIN actors a ON mc.actor_id = a.actor_id
JOIN directors d ON m.director_id = d.director_id
WHERE a.name = 'Natalie Portman'
AND m.release_year BETWEEN 2010 AND 2020
AND mc.role = 'star';
```

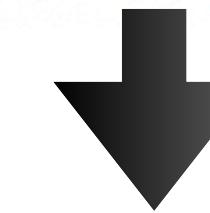
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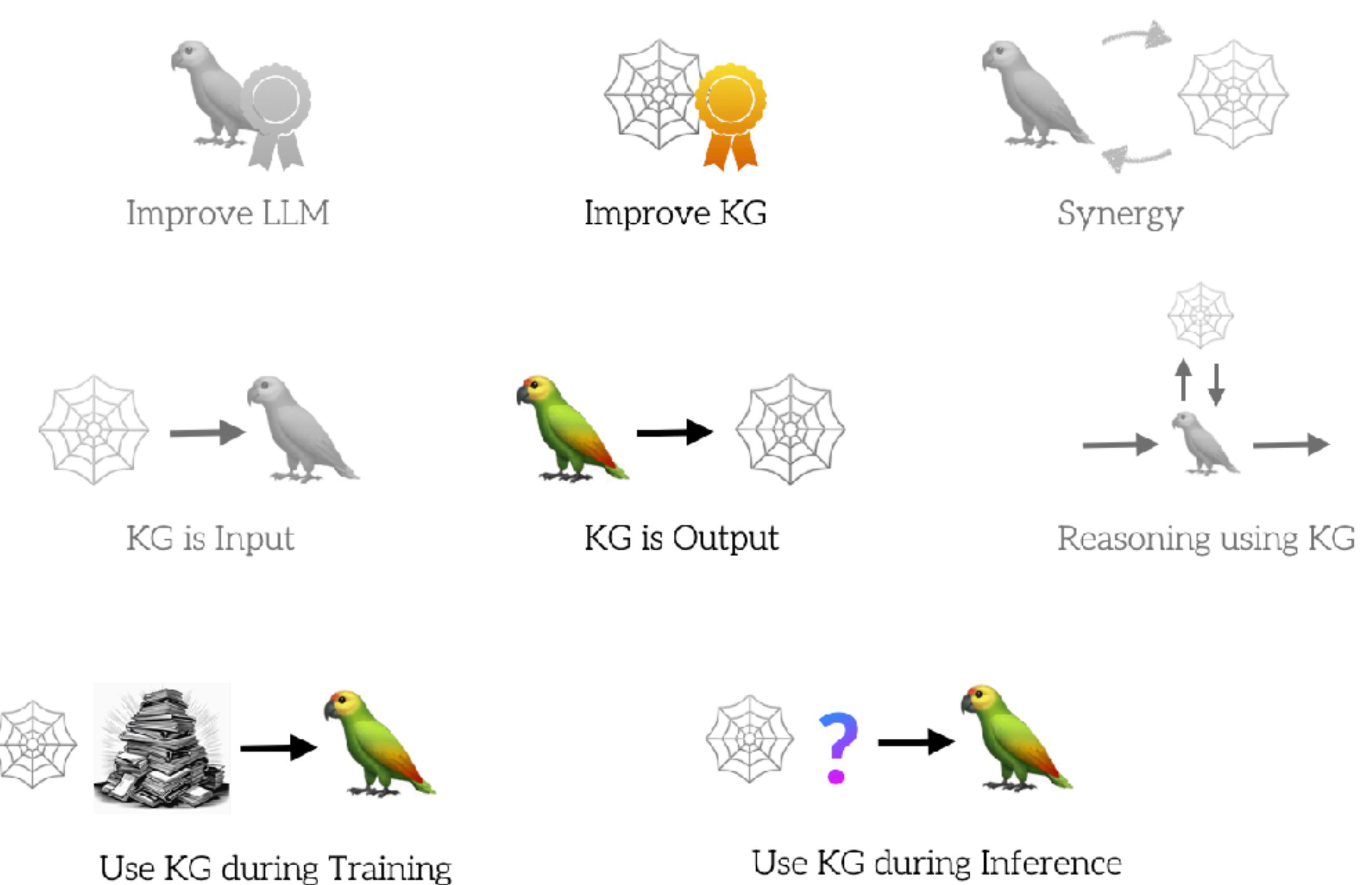


```
MATCH (a:Actor {name: "Natalie Portman"})-[:ACTED_IN]->
(m:Movie)-[:DIRECTED_BY]->(d:Director)
WHERE m.release_year >= 2010 AND m.release_year <= 2020
RETURN DISTINCT d.name AS director_name;
```

KG Completion

Exploring Large Language Models for Knowledge Graph Completion (Yao et al., 2024)

- KGs are (usually) incomplete
- Use LLMs to identify and generate missing links



KG Completion

Exploring Large Language Models for Knowledge Graph Completion (Yao et al., 2024)

Triplet classification: <Steve Jobs, founded, Apple Inc.> => **correct** or **incorrect**

Prompt: *Is this true: Steve Jobs founded Apple Inc.?*

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Entity prediction: <Steve Jobs, ?, Apple Inc.> => **founded**

Prompt: *What is the relationship between Steve Jobs and Apple Inc.?*

Please choose your answer from:

was born in / founded / is citizen of / / plays for

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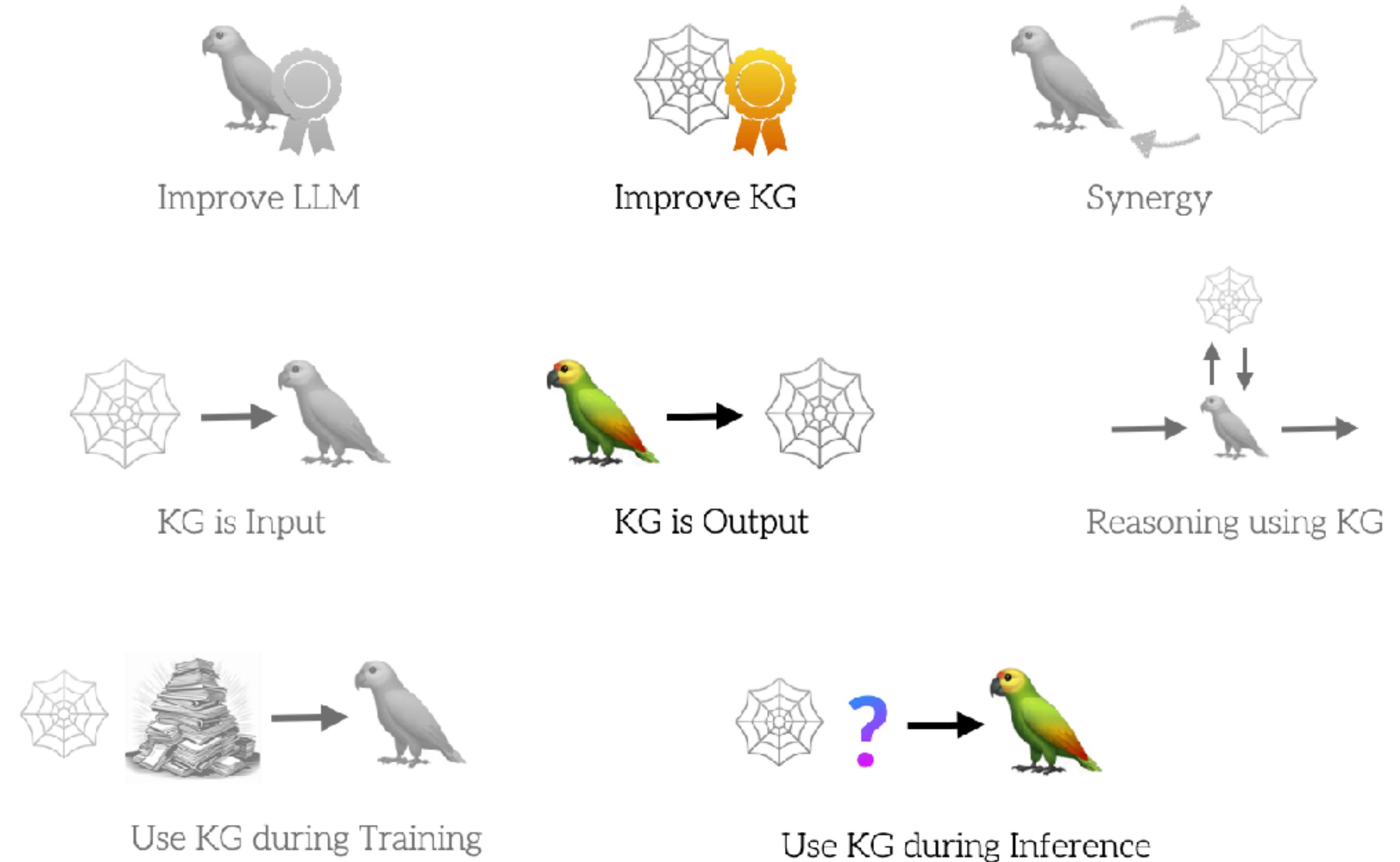
Fine-tuning/Instruction tuning
significantly improves results:

<Steve Jobs, founded, Apple Inc.> → **This is correct.**

KG Construction

Iterative Zero-Shot LLM Prompting for Knowledge Graph Construction (Carta et al., 2023)

- Creating comprehensive and accurate KGs is costly.
- Use zero-shot LLM prompting to extract and organize knowledge.



KG Construction

Iterative Zero-Shot LLM Prompting for Knowledge Graph Construction (Carta et al., 2023)

Candidate Triplet Extraction:

Identify relevant entities and extract their descriptions and type from the text.

(Greatly simplified)

KG Construction

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Resolve ambiguities:

Group the following entities into clusters based on their semantic similarity: Paris, Italy, car, motorbike

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Identify schema:

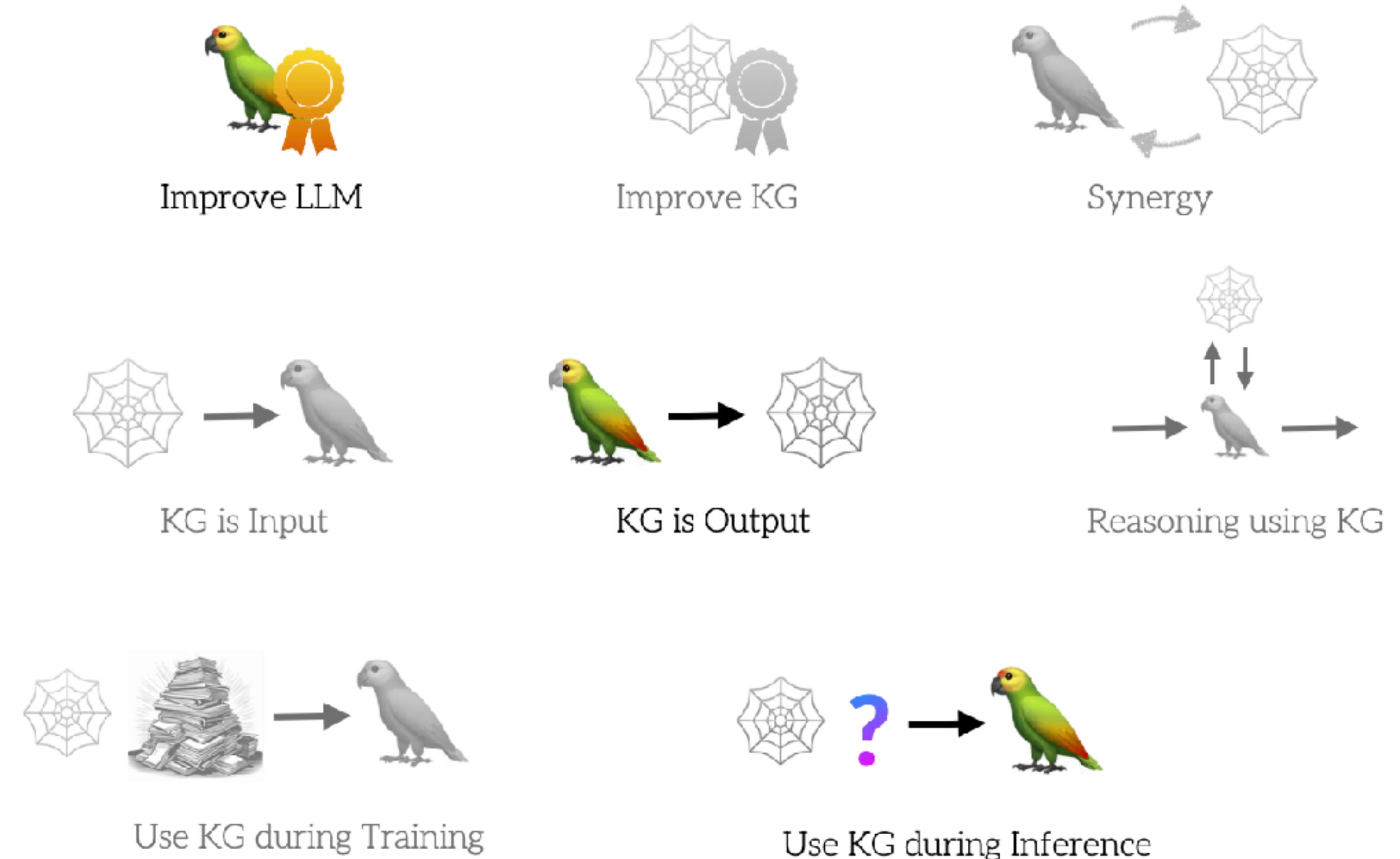
For the following set of entity types, generate a hypernym that can serve as a common category for the entire group: fish, crustacean

(Greatly simplified)

LLM Evaluation

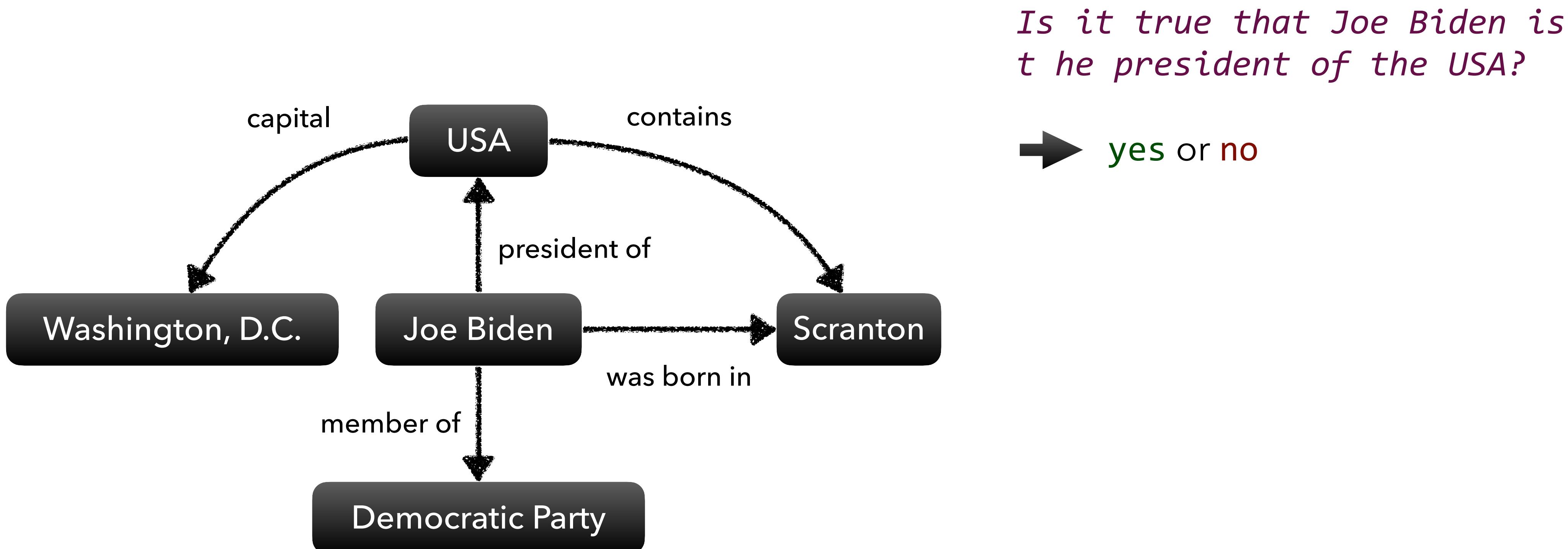
KGLens: Towards Efficient and Effective Knowledge Probing of Large Language Models with Knowledge Graphs (Zheng et al., 2023)

- Evaluating the factualness of LLMs is difficult to scale and adopt.
- Translate KG into natural language questions.
- Identify knowledge blind spots.



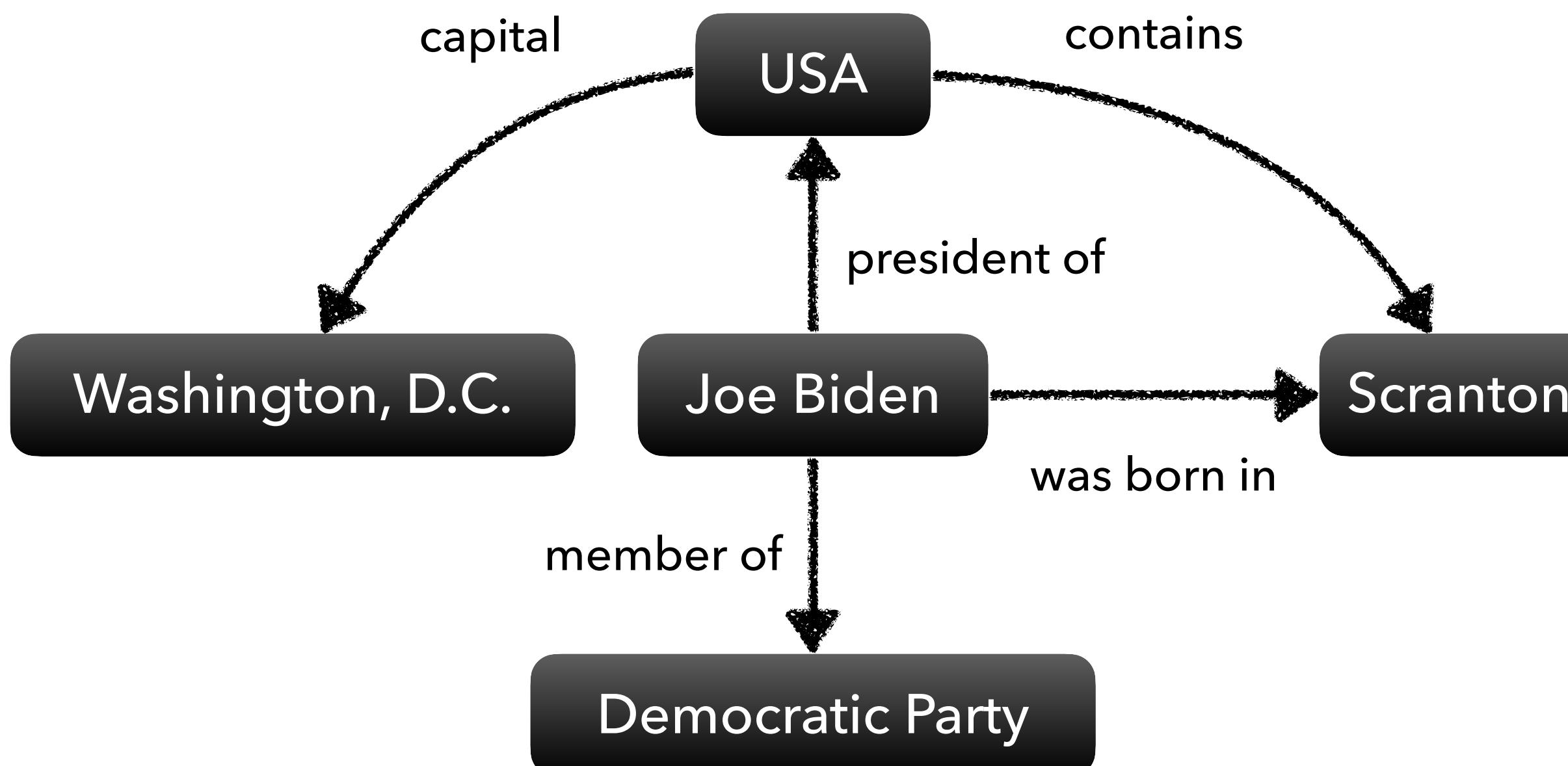
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LLM Evaluation

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Is it true that Joe Biden is the president of the USA?

→ yes or no

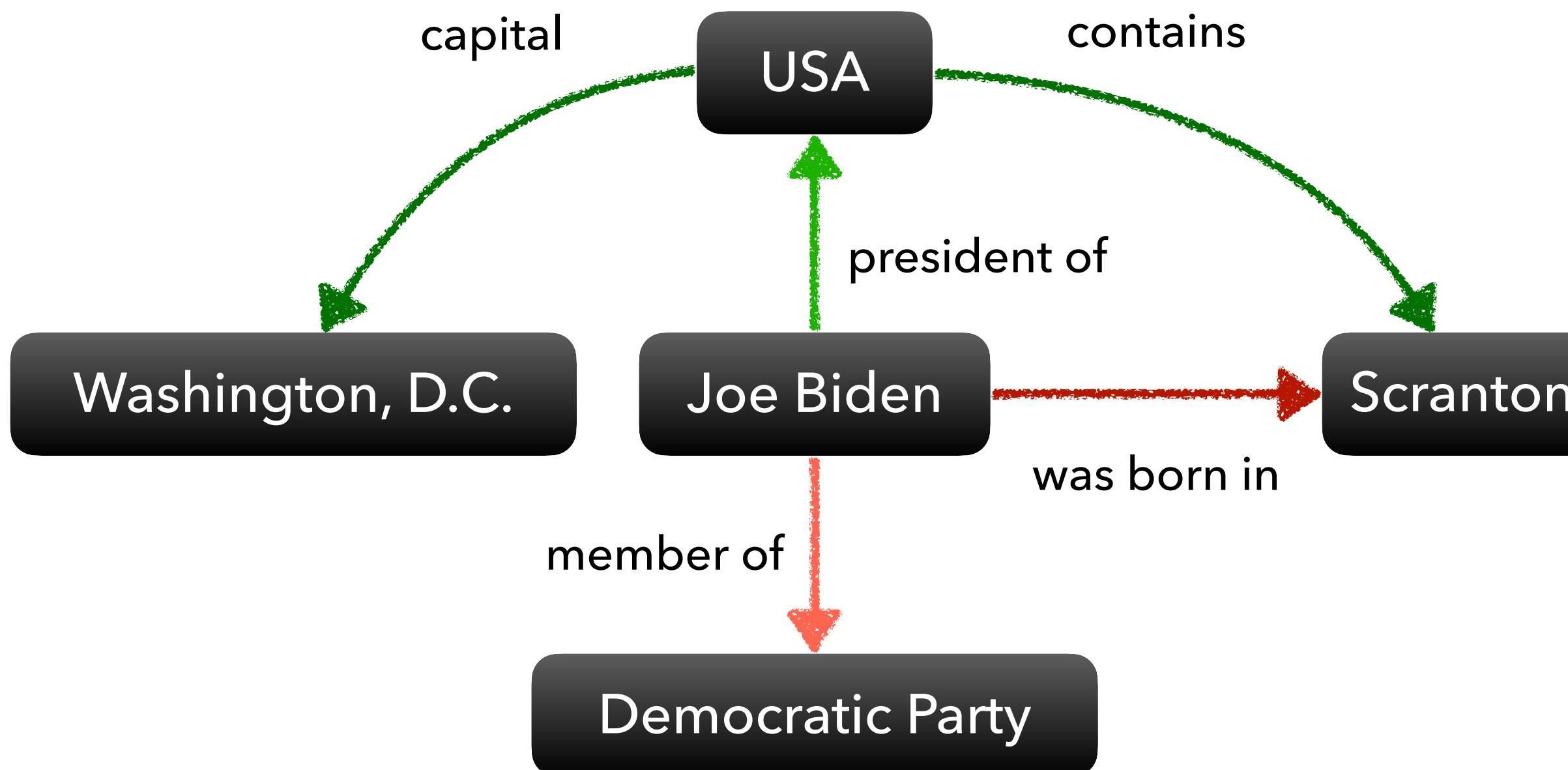
What is the capital of the USA?

→ The capital of the United States of America is Washington, D.C., which stands for the District of Columbia.

- Use LLM to check if the answer matches KG.

LLM Evaluation

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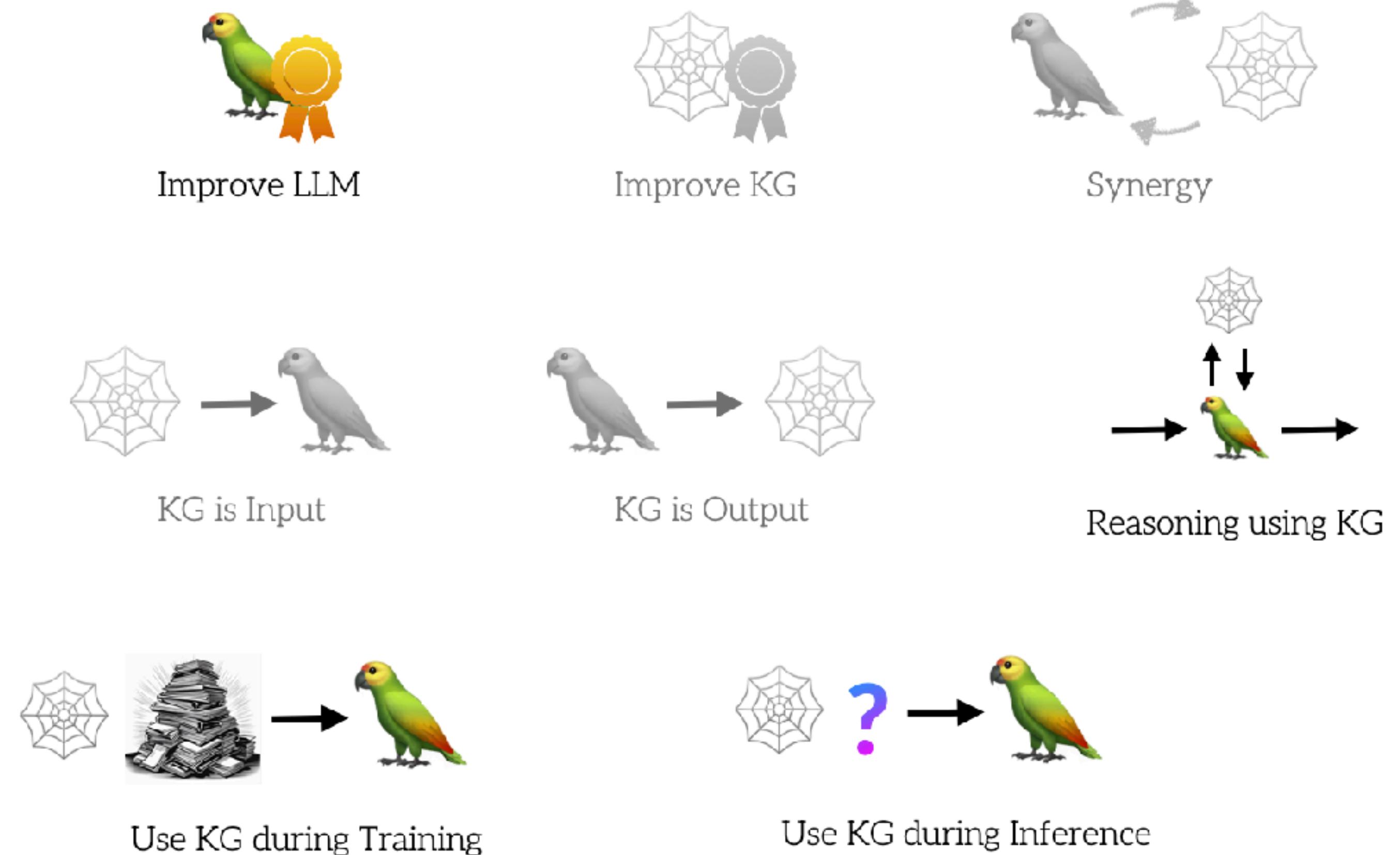


- Estimate likelihood of an LLM failing on each edge.
- Prioritize difficult edges.

Reasoning on Graphs

Reasoning on Graphs: Faithful and Interpretable Large Language Model Reasoning (Luo et al., 2024)

- Lack of (up-to-date) knowledge and hallucinations
- Ground LLM reasoning using KGs



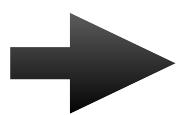
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What is the nationality of Joe Biden?

Generate plan:

*Please generate helpful
relation paths for answering
the question: "What is the
nationality of Joe Biden?"*



<Name> → born in → ? → city of → ?

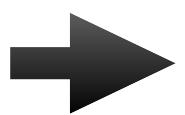
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Retrieve reasoning paths from KGs:

Joe Biden → born in → **Scranton** → city of → **USA**

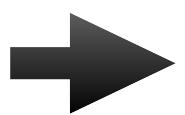
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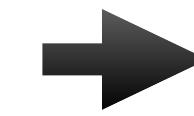
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Answer based on paths:

*Please answer the
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**Joe Biden's nationality
is American since he was
born in the USA.**

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Use fine-tuning to improve results.

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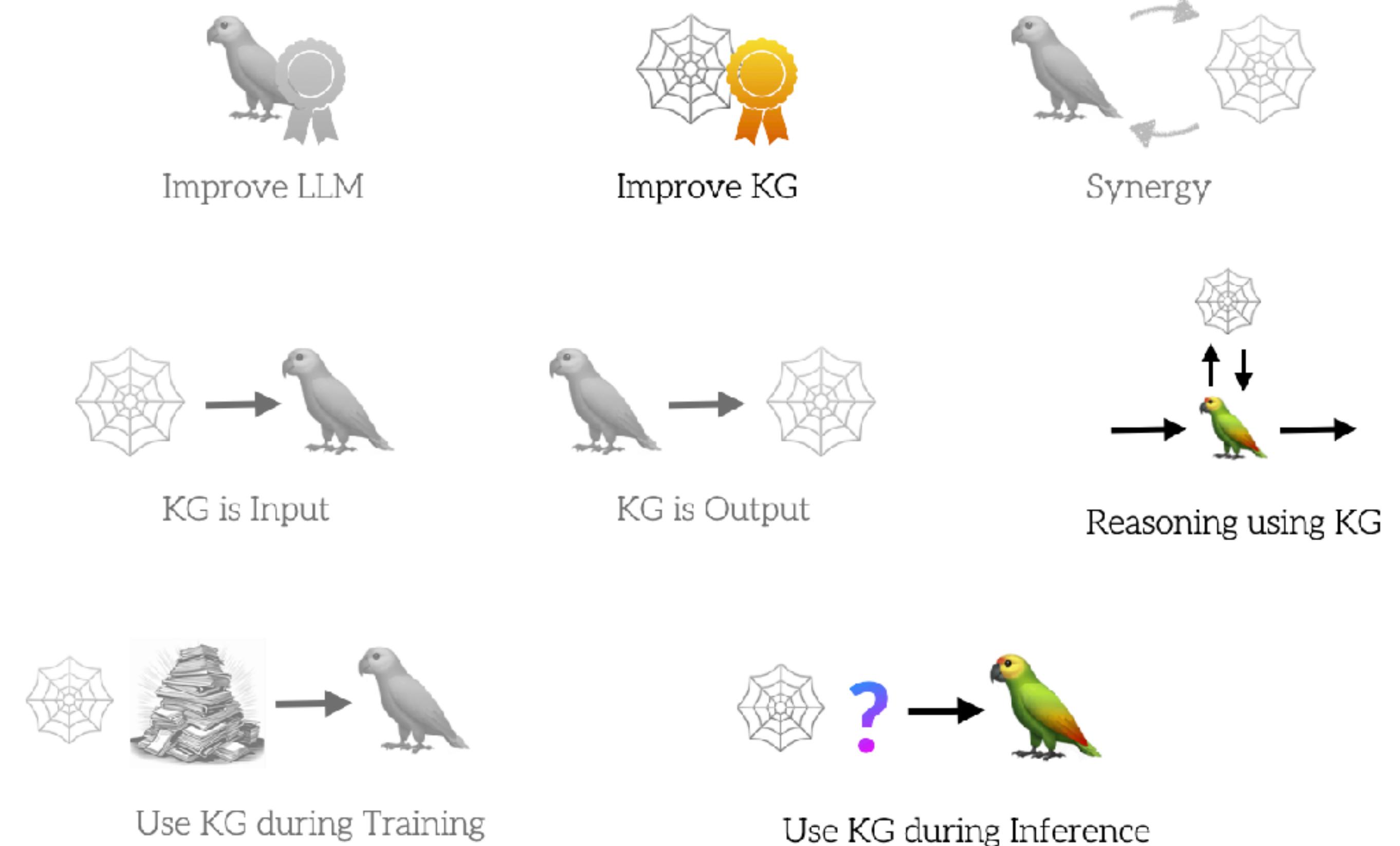


*Joe Biden's nationality
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Reasoning on Graphs II

Graph Language Models (Plenz et al., 2024)

- Feeding KGs as triplets to LLMs is very inefficient
- Combine Graph Neural Network with LLM

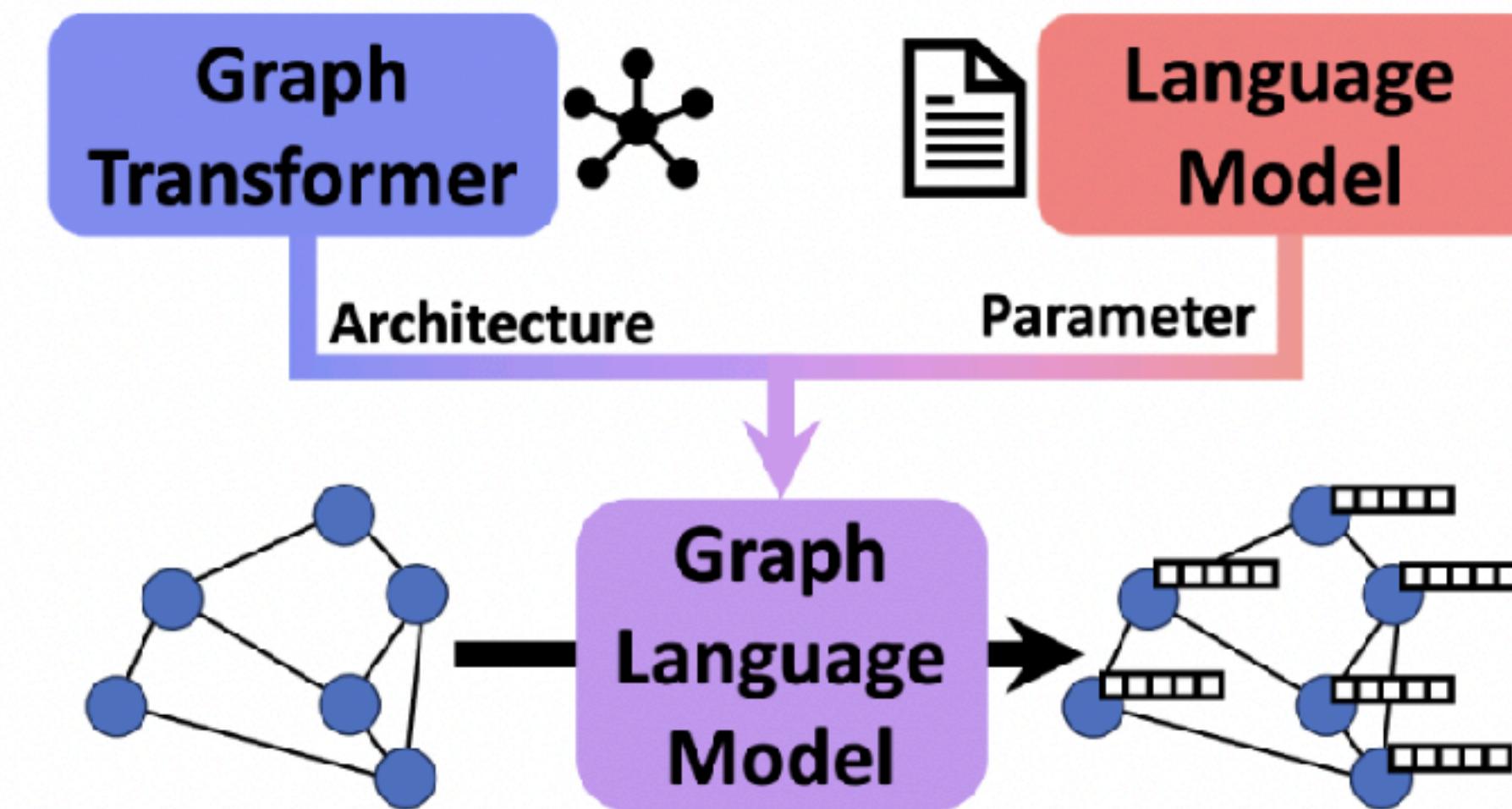


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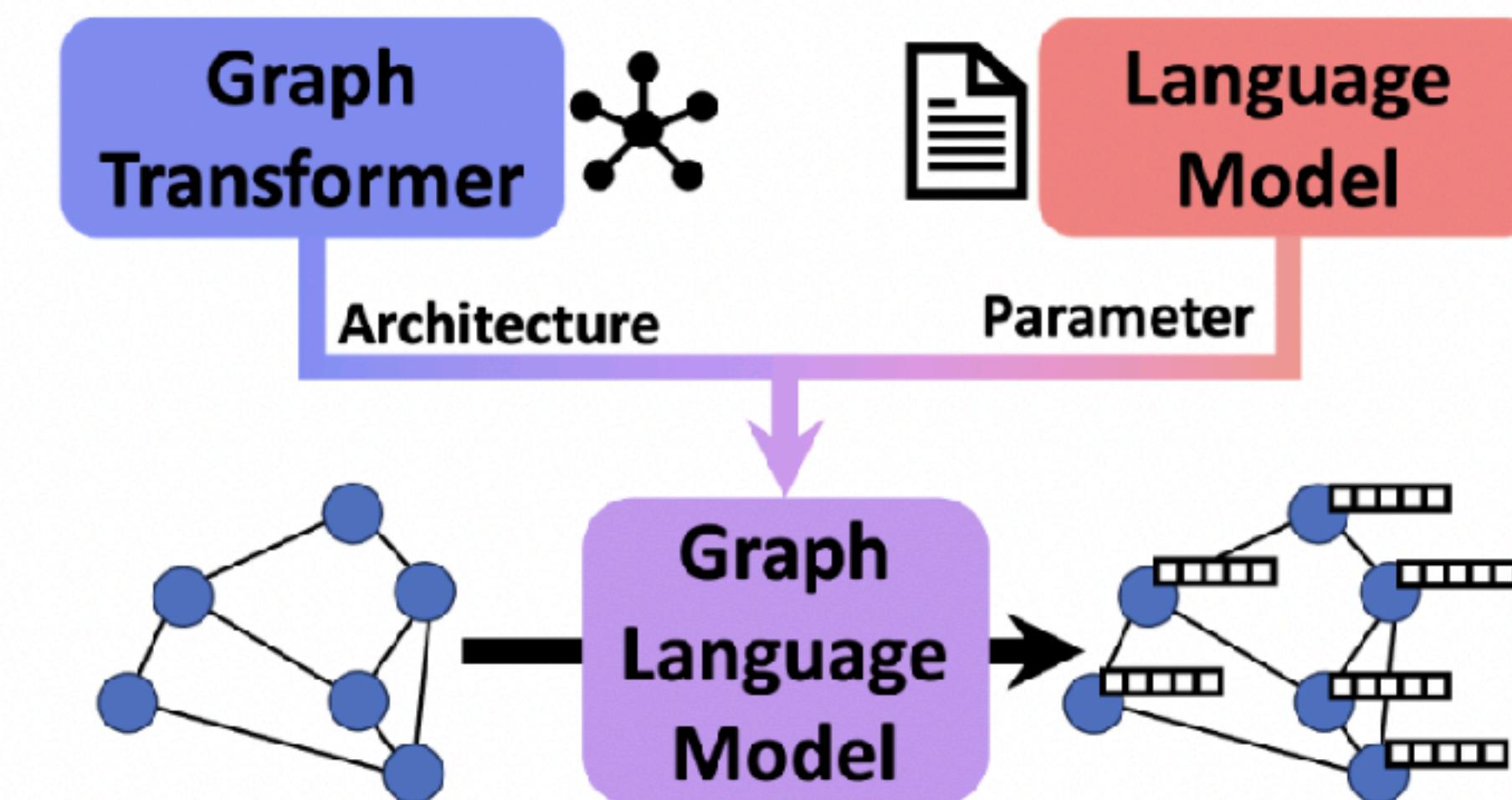


Reasoning on Graphs II

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“[W]e transform the LM to a Graph Transformer (GT) – while maintaining compatibility with its pretrained LM parameters.”

- Add a GNN mechanism to a LLM
 - ▶ requires graph-based positional embeddings
- Use GNN + LLM parameters to reason over KG



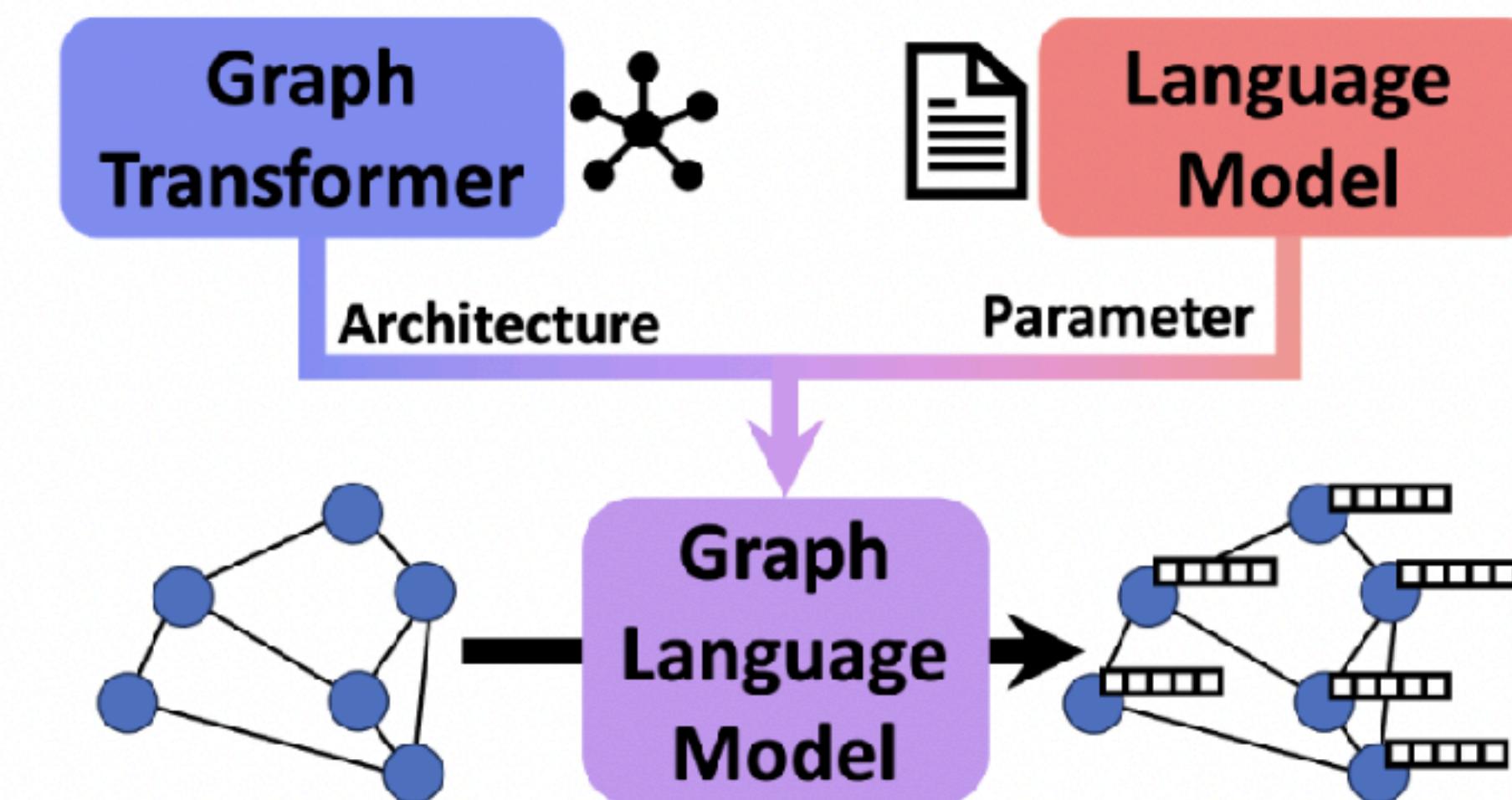
Entity prediction: <Steve Jobs, ?, Apple Inc.> => founded

Reasoning on Graphs II

Graph Language Models (Plenz et al., 2024)

“[W]e transform the LM to a Graph Transformer (GT) – while maintaining compatibility with its pretrained LM parameters.”

- Add a GNN mechanism to a LLM
 - ▶ requires graph-based positional embeddings
- Use GNN + LLM parameters to reason over KG
- T5 (only use the encoder)

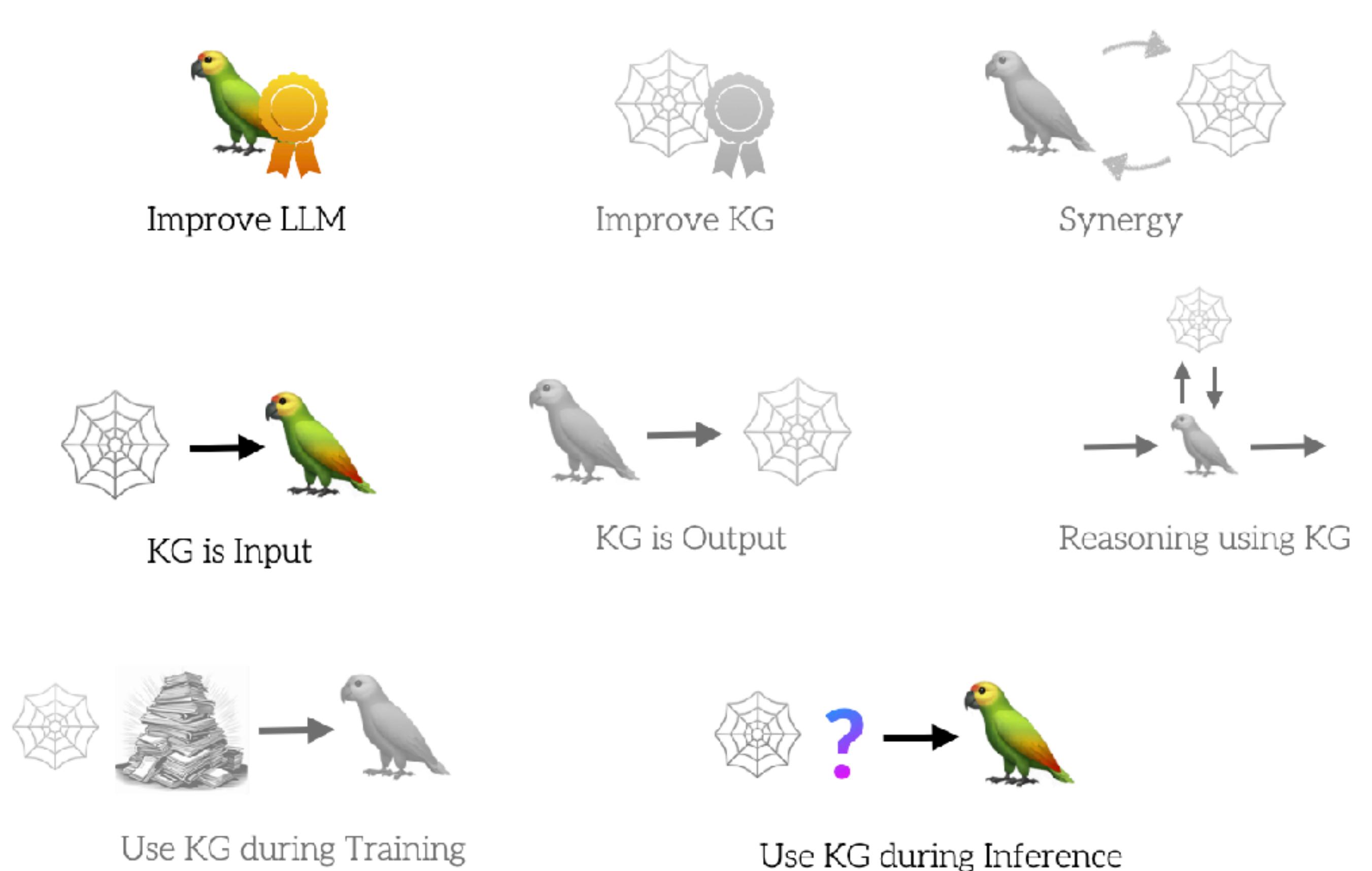


Entity prediction: <Steve Jobs, ?, Apple Inc.> => founded

Retrofitting KGs

Mitigating Large Language Model Hallucinations via Autonomous Knowledge Graph-based Retrofitting
(Guan et al., 2023)

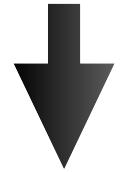
- Verify the LLM response based on a KG.
- Adjust it if incorrect.



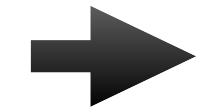
Retrofitting KGs

Mitigating Large Language Model Hallucinations via Autonomous Knowledge Graph-based Retrofitting
(Guan et al., 2023)

What is the capital of the USA?



The capital of the USA is NYC.

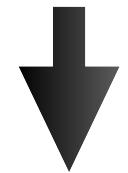


New York City → is capital of → **USA**

Retrofitting KGs

Mitigating Large Language Model Hallucinations via Autonomous Knowledge Graph-based Retrofitting
(Guan et al., 2023)

What is the capital of the USA?



The capital of the USA is NYC.

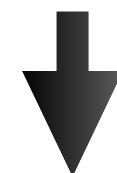


New York City → is capital of → **USA**

The capital of the USA is Washington, D.C.

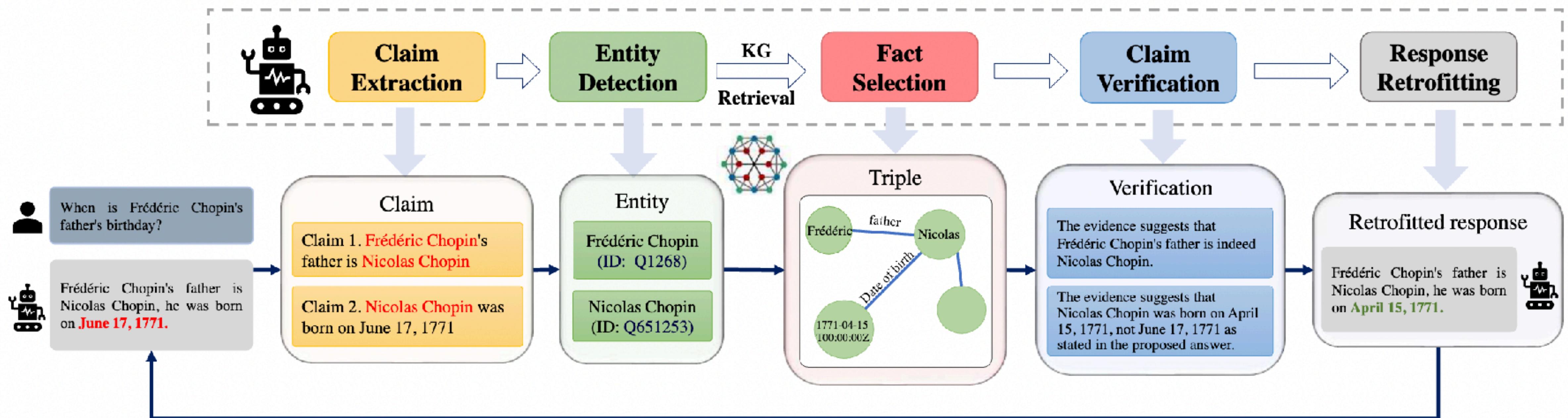


Washington, D.C. → is capital of → **USA**



Retrofitting KGs

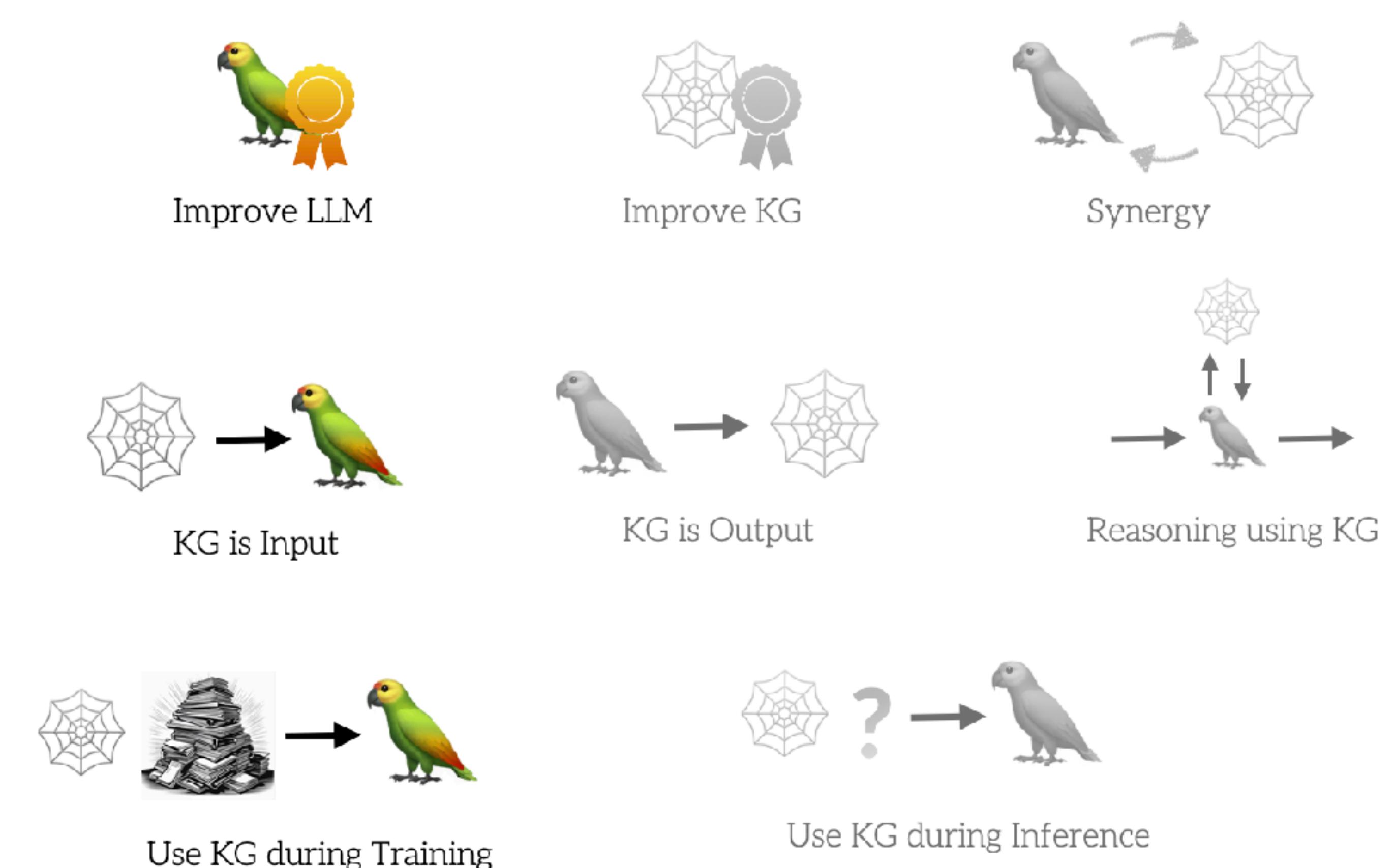
Mitigating Large Language Model Hallucinations via Autonomous Knowledge Graph-based Retrofitting
(Guan et al., 2023)



Training on KGs

SKILL: Structured Knowledge Infusion for Large Language Models (Moiseev, 2022)

- Convert KG into text to use as training data.
- Enhance LLM performance wrt. factual knowledge.



Training on KGs

SKILL: Structured Knowledge Infusion for Large Language Models (Moiseev, 2022)

(Washington, D.C., is capital of, USA)

Option 1: Train directly on triplet

(Washington D.C., [mask], USA)

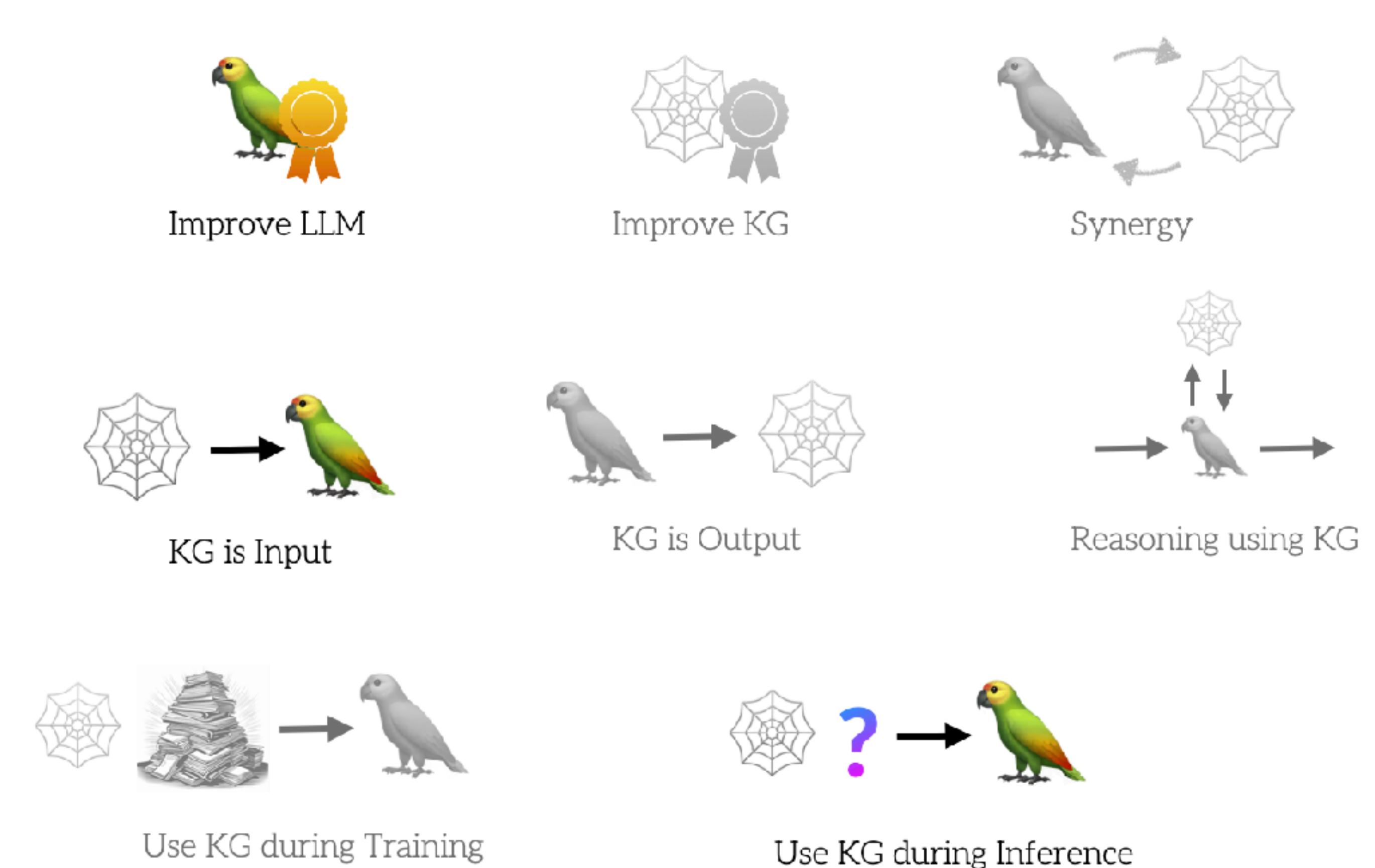
Option 2: Convert to text

Washington, D.C. is the capital of the USA.

Both methods work well.

KG as Input

- Fine-tuning is often too expensive.





Part III

Knowledge Graphs for Retrieval Augmented Generation

RAG Recap

How much money did I spend on coffee last week?

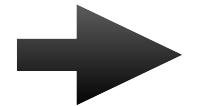


Idk.

How much money did I spend on coffee last week?



*Given these financial records:
(3.50 EUR, Cappuccino, 12.08.2024)
(2.80 EUR, Espresso, 15.08.2024)
(2.30 EUR, Cortado, 19.08.2024)*



8,60 EUR.

*Answer the question:
How much money did I spend on coffee last week?*

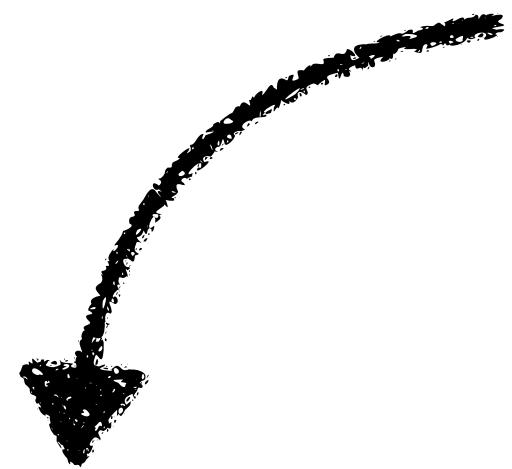
RAG Recap

- We assume there is a corresponding dataset.
 - ▶ private,
 - ▶ up-to-date
 - ▶ specialized
- Challenge: Identify the relevant entries.

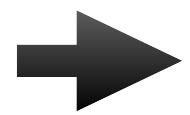
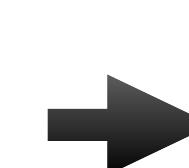
How much money did I spend on coffee last week?



Given these financial records:
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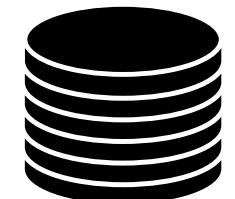


Answer the question:
How much money did I spend on coffee last week?

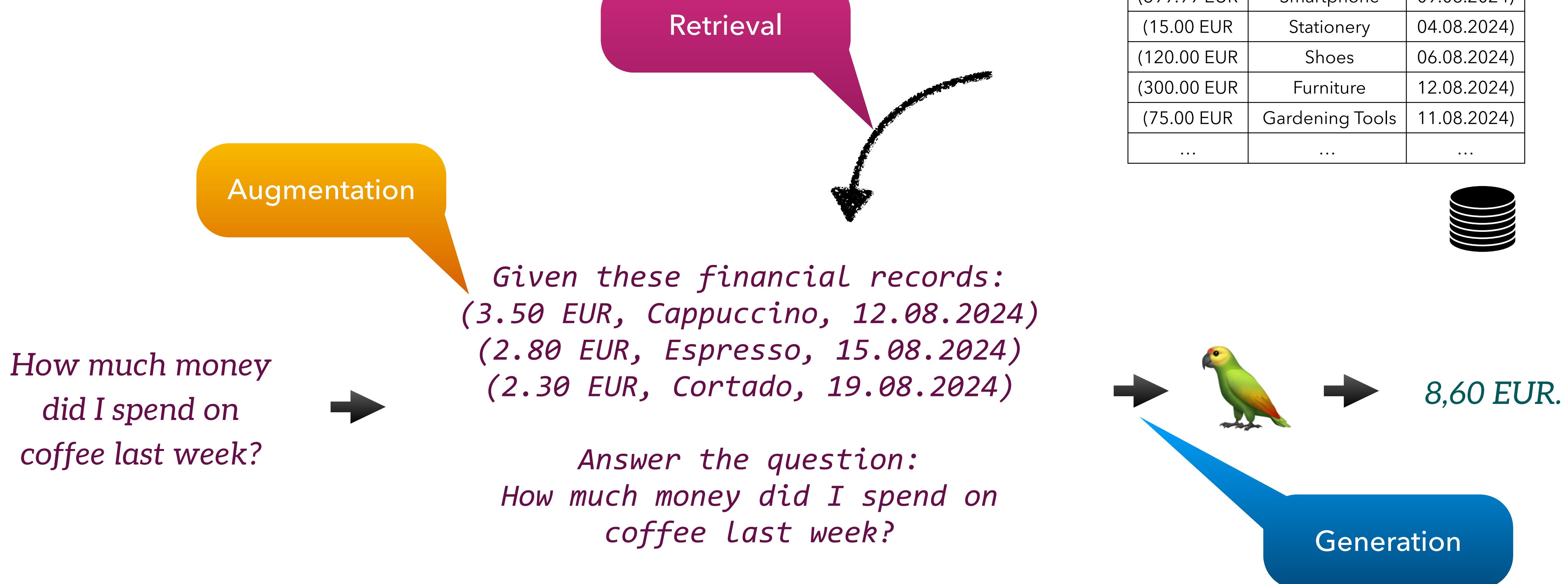


8,60 EUR.

(899.99 EUR	New TV	07.08.2024)
(45.00 EUR	Plants	10.08.2024)
(25.50 EUR	Books	02.08.2024)
(60.00 EUR	Clothing	08.08.2024)
(29.99 EUR	Kitchen Utensils	03.08.2024)
(399.99 EUR	Smartphone	09.08.2024)
(15.00 EUR	Stationery	04.08.2024)
(120.00 EUR	Shoes	06.08.2024)
(300.00 EUR	Furniture	12.08.2024)
(75.00 EUR	Gardening Tools	11.08.2024)
...



RAG Recap



RAG Recap

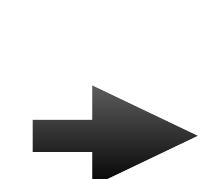
How much money
did I spend on
coffee last week?



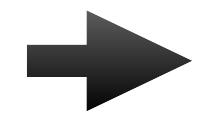
Dataset can also be a KG.



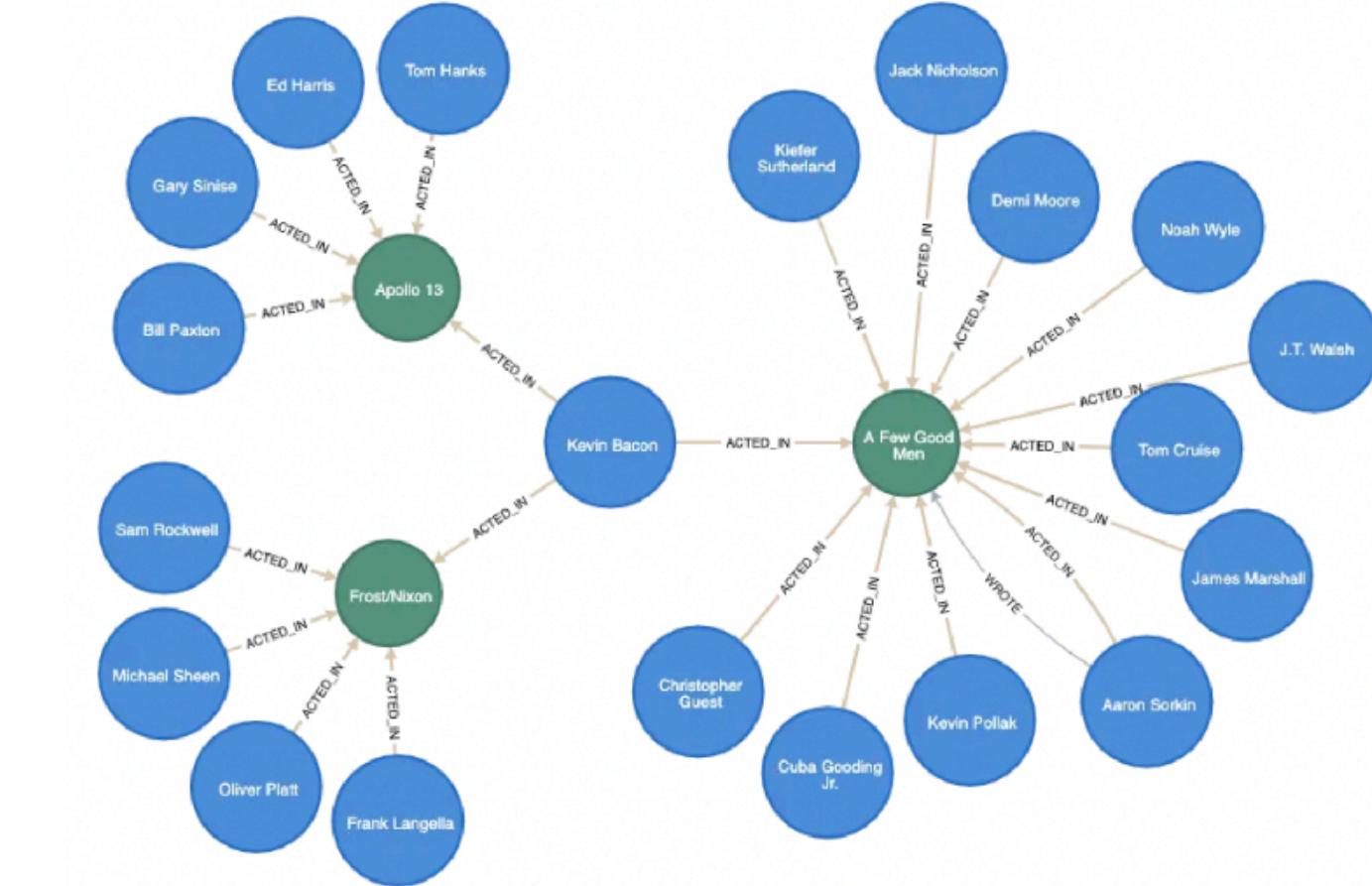
Given these financial records:
(3.50 EUR, Cappuccino, 12.08.2024)
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Answer the question:
*How much money did I spend on
coffee Last week?*



8,60 EUR.



RAG Recap

How much money
did I spend on
coffee last week?



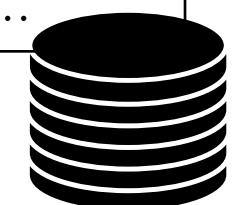
Challenge: Identify the
relevant entries.



Given these financial records:
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Answer the question:
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(300.00 EUR	Furniture	12.08.2024)
(75.00 EUR	Gardening Tools	11.08.2024)
...



8,60 EUR.

RAG Recap

1) Embedding

acting as

Vector Index



How much money
did I spend on
coffee last week?



Given these financial records:
(3.50 EUR, Cappuccino, 12.08.2024)
(2.80 EUR, Espresso, 15.08.2024)
(2.30 EUR, Cortado, 19.08.2024)



8,60 EUR.

Answer the question:
*How much money did I spend on
coffee last week?*

RAG Recap

2) Identify entries

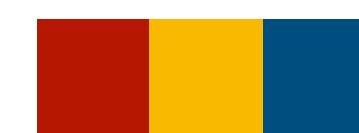
with **similar**

embeddings in **vector**

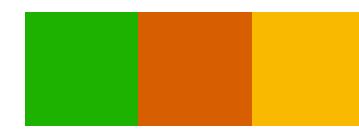
database.



Gardening Tools



Espresso



Shoes



Cappuccino



New TV



Plants



Cortado

1) Embedding

acting as

Vector Index



How much money
did I spend on
coffee last week?



Given these financial records:
(3.50 EUR, Cappuccino, 12.08.2024)
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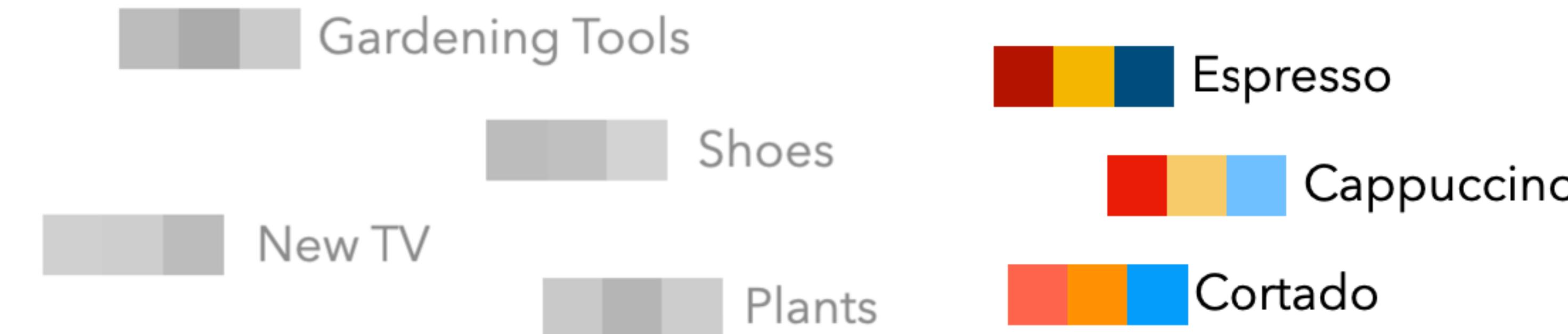


8,60 EUR.

Answer the question:
*How much money did I spend on
coffee Last week?*

RAG Recap

2) Identify entries
with **similar**
embeddings in **vector**
database.



1) Embedding
acting as
Vector Index



How much money
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coffee last week?



Given these financial records:
(3.50 EUR, Cappuccino, 12.08.2024)
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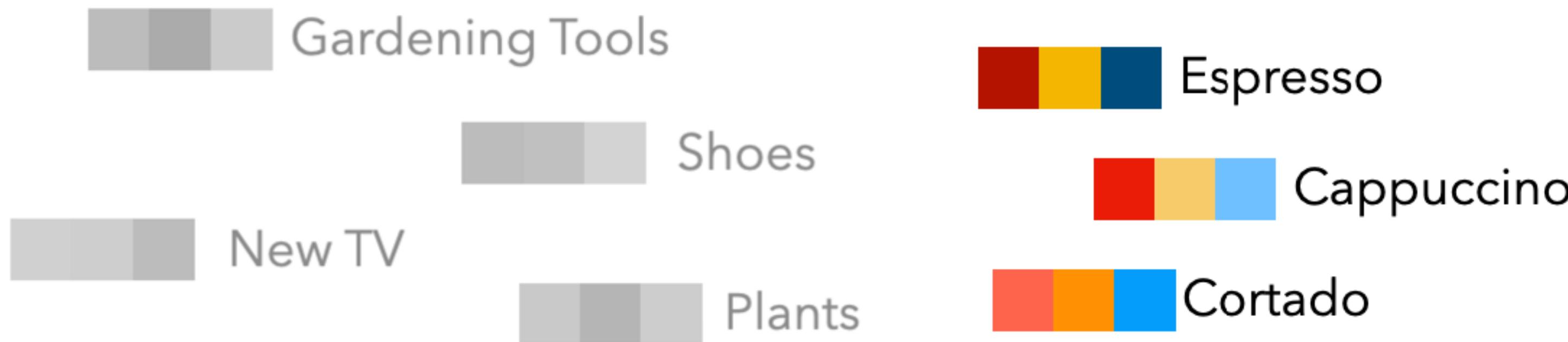


8,60 EUR.

Answer the question:
*How much money did I spend on
coffee last week?*

RAG Recap

2) Identify entries
with **similar**
embeddings in **vector**
database.



1) **Embedding**
acting as
Vector Index



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Given these financial records:
(3.50 EUR, Cappuccino, 12.08.2024)
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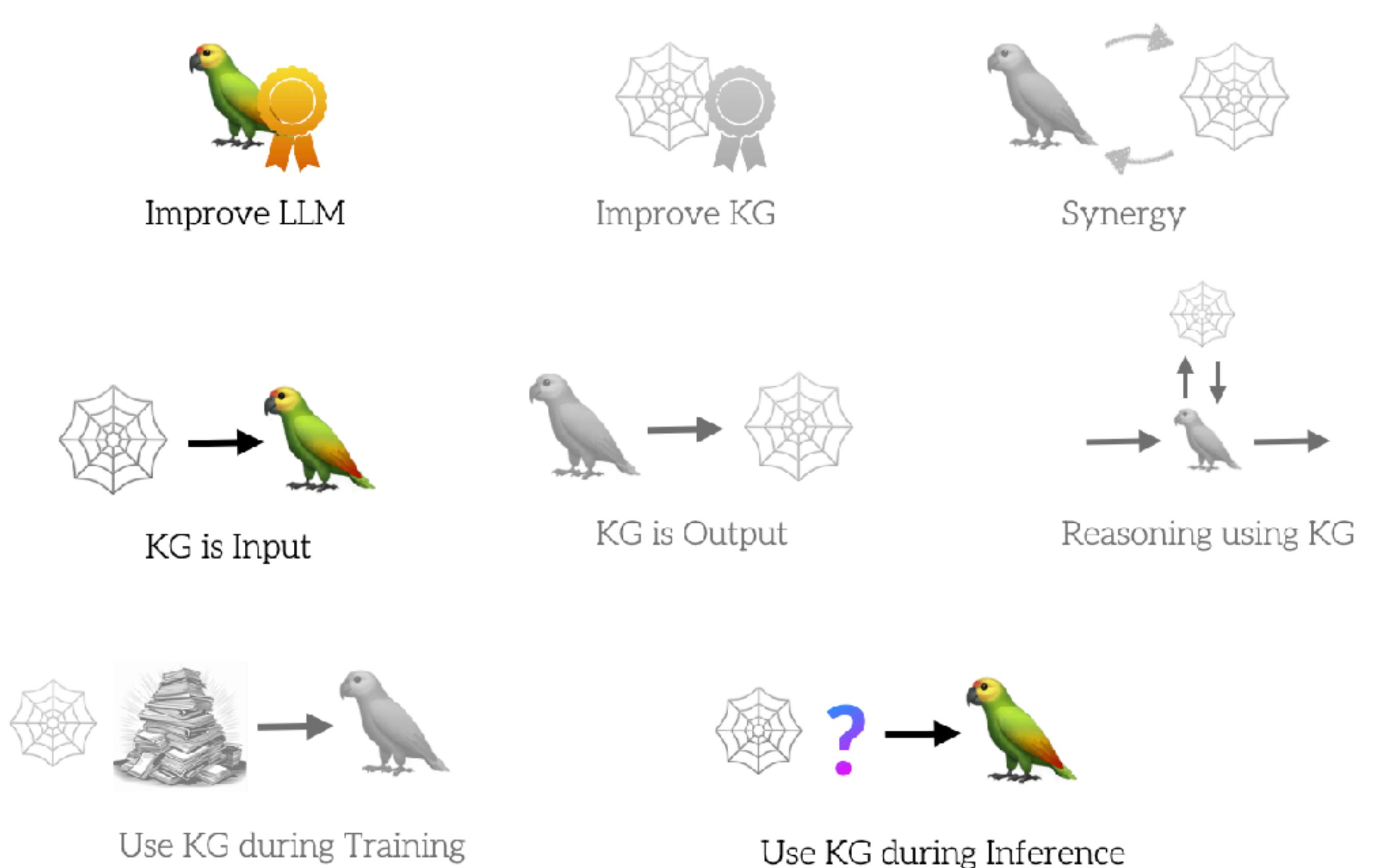
8,60 EUR.

Answer the question:
How much money did I spend on
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KG-Based RAG

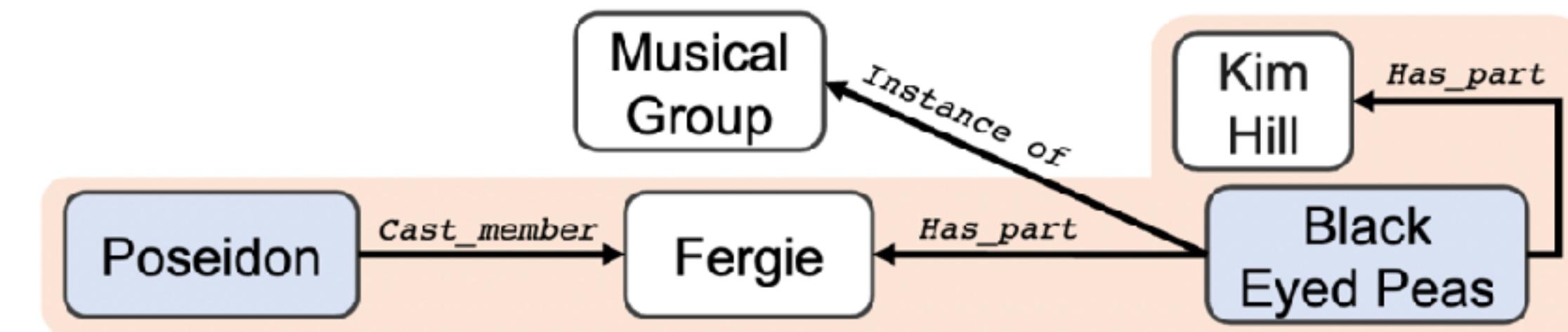
Knowledge-Augmented Language Model Prompting for Zero-Shot Knowledge Graph Question Answering
(Baek et al., 2023)

- Augment the input of LLMs with relevant facts retrieved from a knowledge graph.



KG-Based RAG

Knowledge-Augmented Language Model Prompting for Zero-Shot Knowledge Graph Question Answering
(Baek et al., 2023)

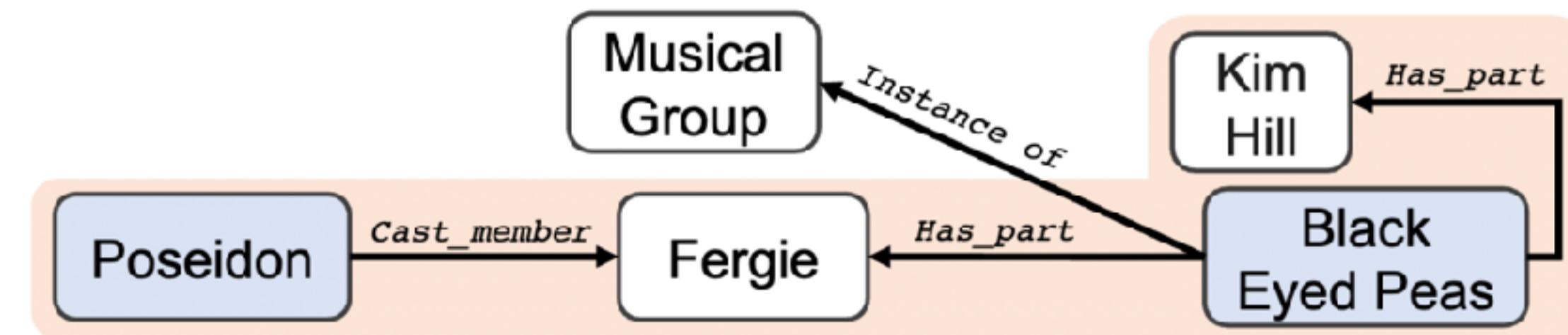


*Which member of Black
Eyed Peas appeared in
Poseidon?*



KG-Based RAG

Knowledge-Augmented Language Model Prompting for Zero-Shot Knowledge Graph Question Answering
(Baek et al., 2023)



Below are the facts that might be relevant to answer the question:

*(Black Eyed Peas, has part, Fergie),
(Black Eyed Peas, has part, Kim Hill),
(Poseidon, cast member, Fergie)*

*Question:
Which member of Black Eyed Peas appeared in Poseidon? Answer:*

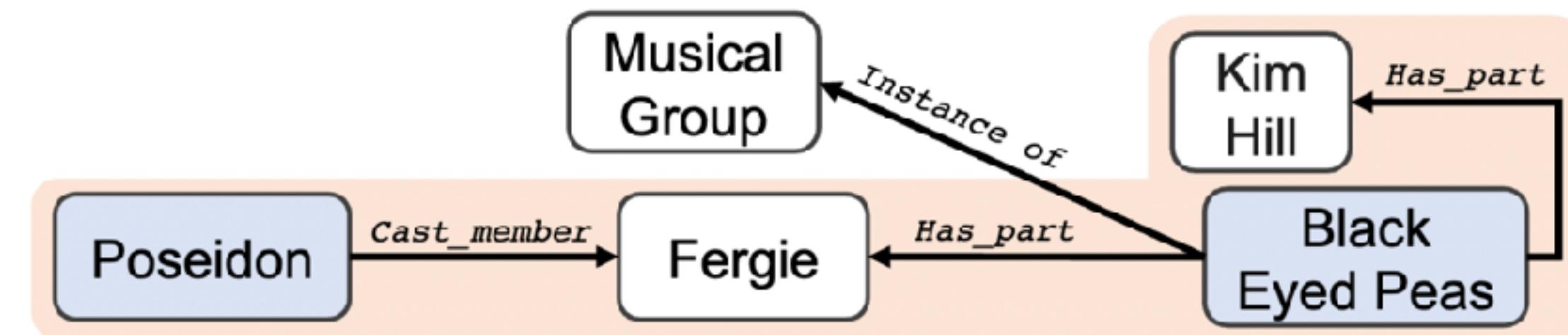
Which member of Black Eyed Peas appeared in Poseidon?



Fergie

KG-Based RAG

Knowledge-Augmented Language Model Prompting for Zero-Shot Knowledge Graph Question Answering
(Baek et al., 2023)



Entity extraction/matching
+ embedding similarity

Which member of Black Eyed Peas appeared in Poseidon? →

Below are the facts that might be relevant to answer the question:

*(Black Eyed Peas, has part, Fergie),
(Black Eyed Peas, has part, Kim Hill),
(Poseidon, cast member, Fergie)*

*Question:
Which member of Black Eyed Peas appeared in Poseidon? Answer:*

→ *Fergie*

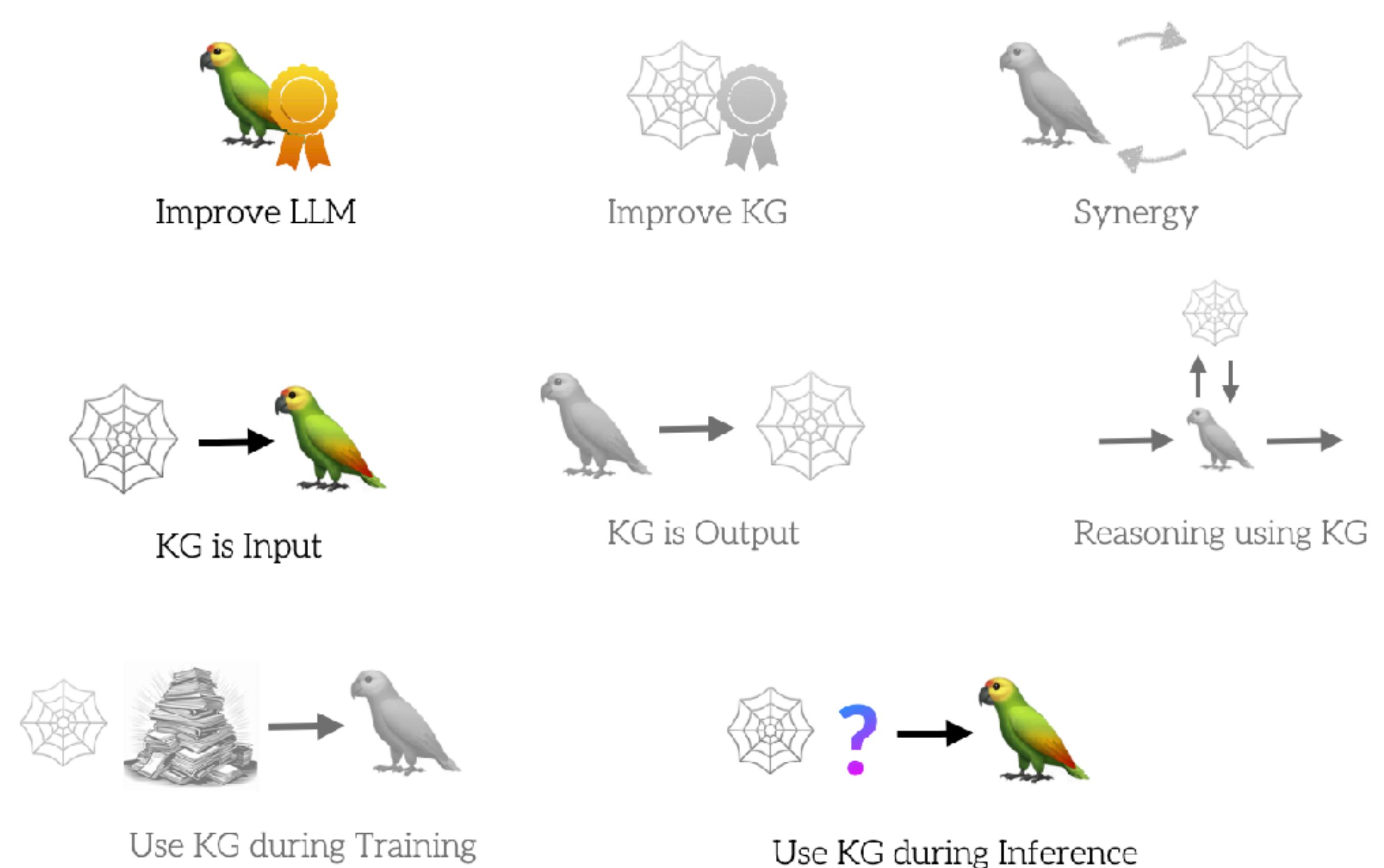
KG-Based RAG

From Local to Global: A Graph RAG Approach to Query-Focused Summarization (Edge et al., 2024)

- **(Vanilla) RAG struggles with global questions:**

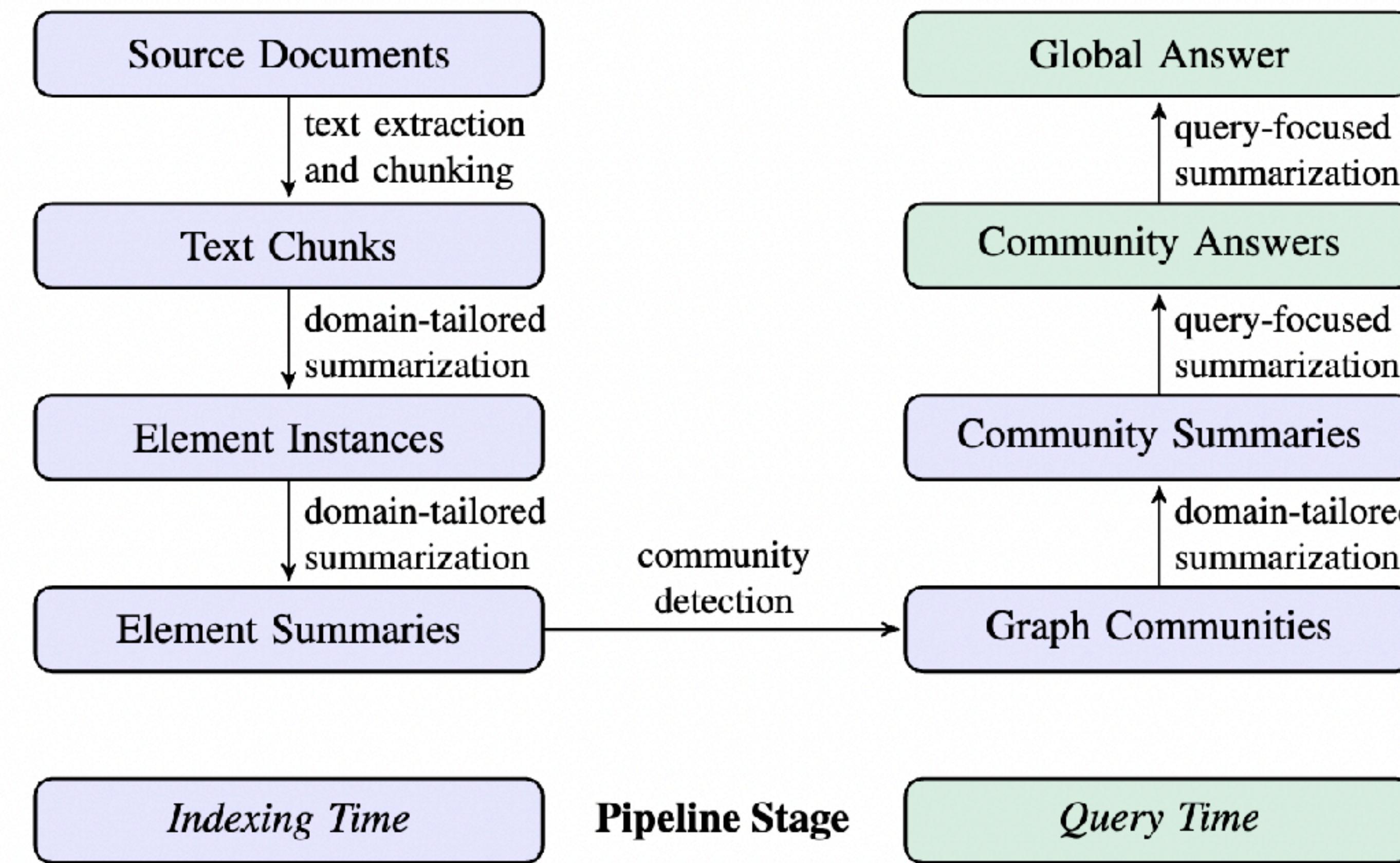
„What are the main themes in the dataset?“

- **Convert dataset to KG + exploit graph structure for retrieval.**



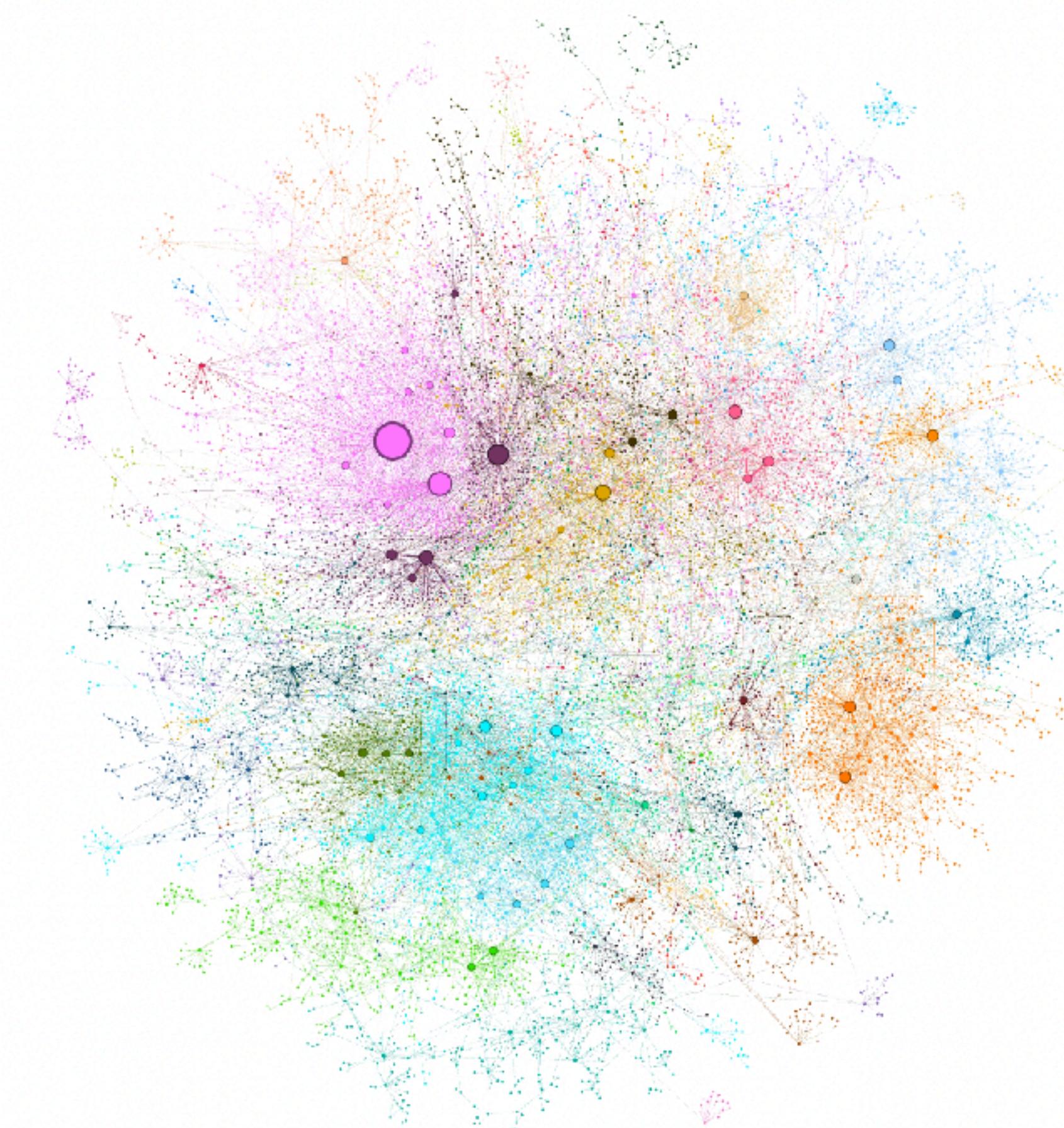
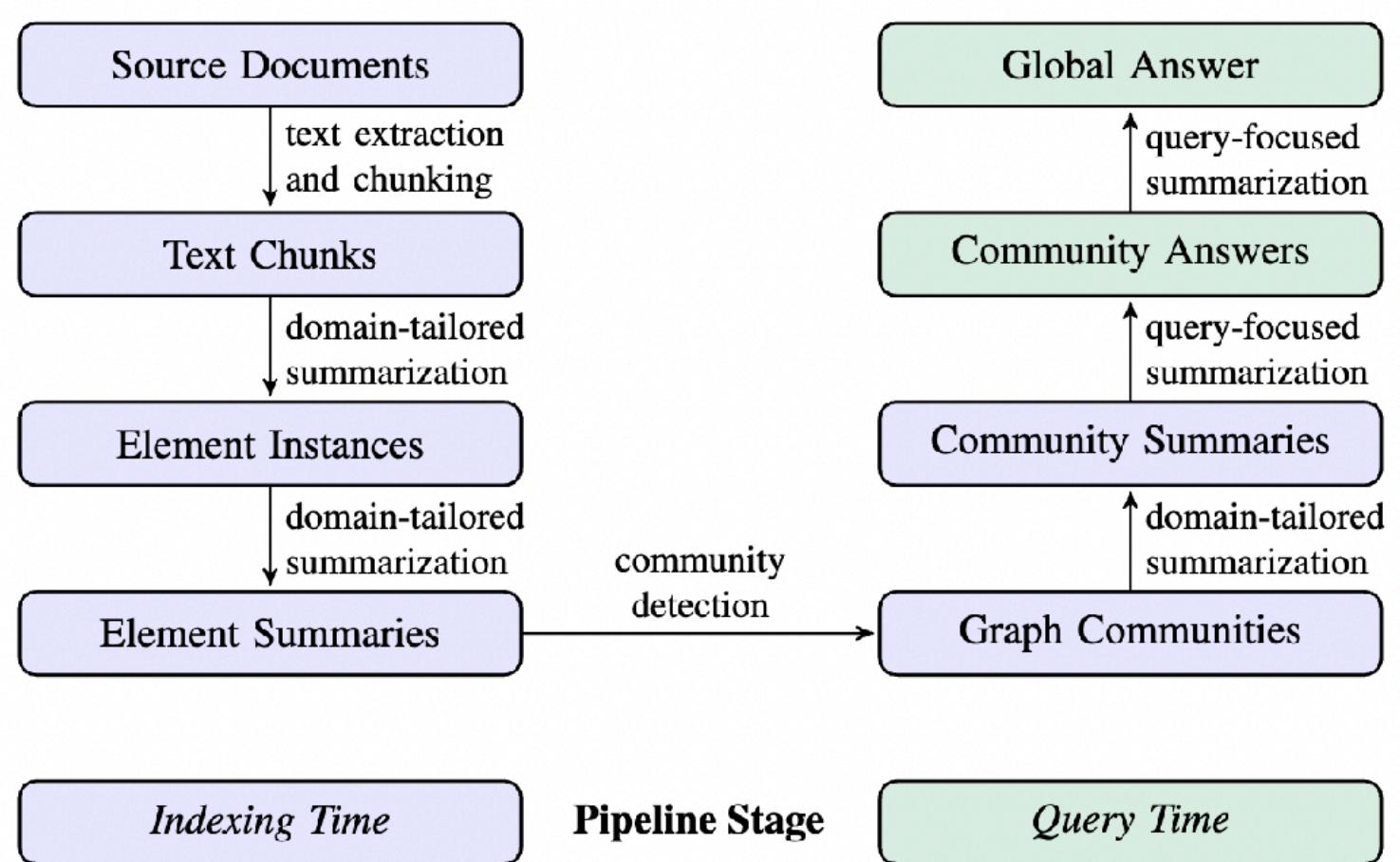
KG-Based RAG

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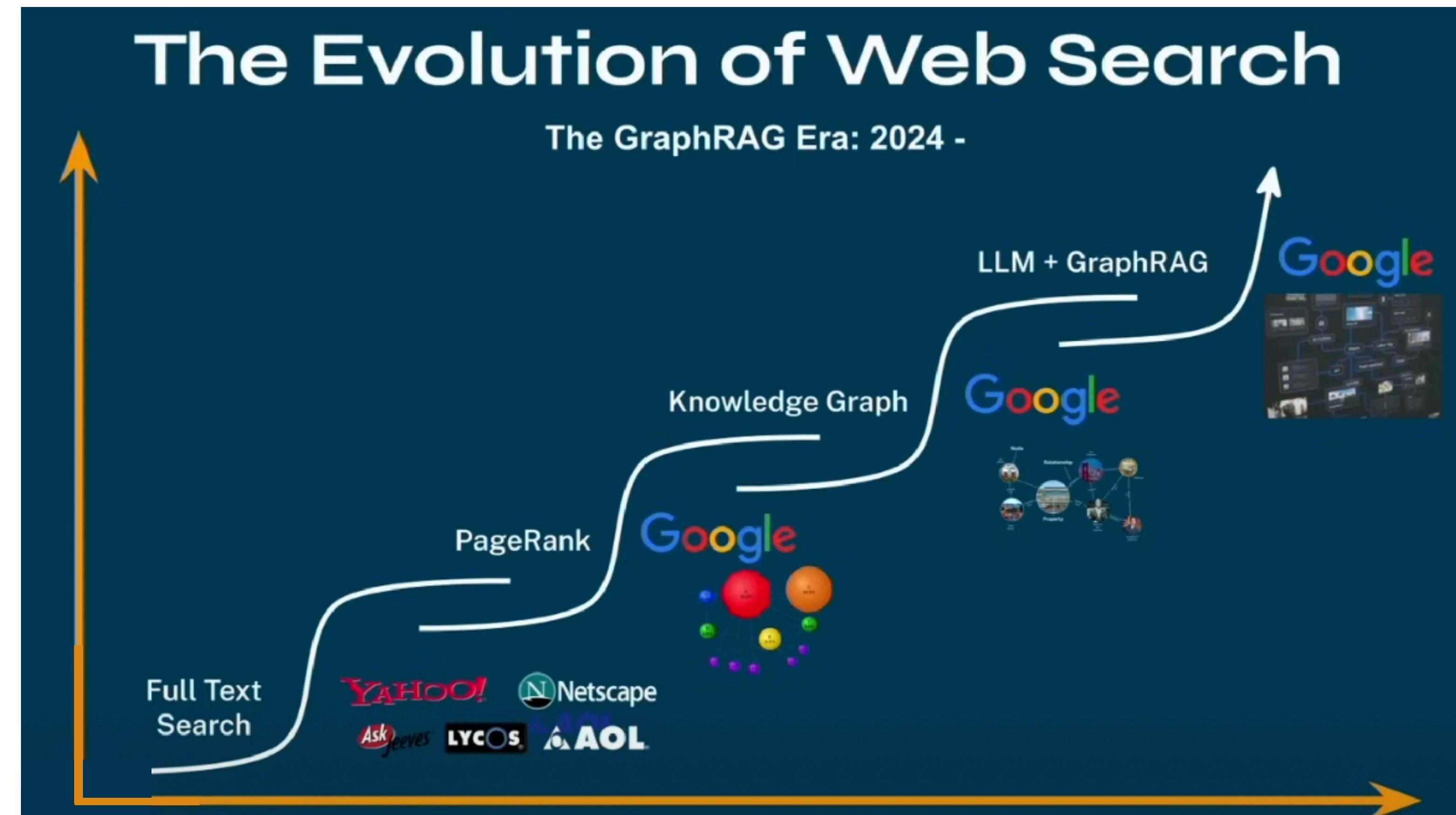


KG-Based RAG

From Local to Global: A Graph RAG Approach to Query-Focused Summarization (Edge et al., 2024)



Outlook



Build Your Own GraphRAG



Ollama



LitGPT



OpenAI



Amazon



HuggingFace



Neo4j



NebulaGraph



LangChain



Llamaindex

Main LLM

Embedding LLM

Graph database

Toolchain

Build Your Own GraphRAG



Ollama



LitGPT



OpenAI



Amazon



HuggingFace



Neo4j



NebulaGraph



LangChain



LlamalIndex

Main LLM

Embedding LLM

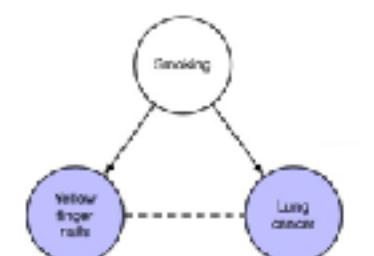
Graph database

Toolchain

Generate KG:

- Create your own KG manually
- Neo4J: LLM graph builder
- Microsoft GraphRAG
- LlamalIndex: KnowledgeGraphIndex

Summary

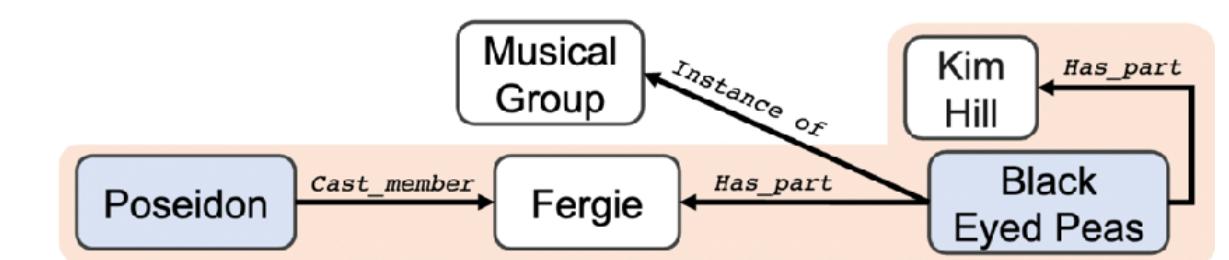


Everything is a graph.

KGs can improve LLMs.
LLMs can improve KGs.



RAG equips LLMs with
real-time and private data.



Graph RAG =
Higher accuracy + global answers

We are hiring:

dataciapps.de/jobs

All references are available on:

github.com/gerritgr/LLMSummerSchool



References

Surveys:

- Unifying Large Language Models and Knowledge Graphs: A Roadmap (Pan et al., 2023)
- Graph Machine Learning in the Era of Large Language Models (Fan et al., 2024)

Tutorials:

- ArangoDB - LLMS With Knowledge Graph (youtube.com/watch?v=DkbX8O9zd_8)
- AI Engineer World's Fair 2024 (talk by Emil Eifrem highly recommended)
- Neo4j Graphacademy
- ACL 2023 Tutorial: Complex Reasoning in Natural Language (wenting-zhao.github.io/complex-reasoning-tutorial/)

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