TKDE23: Unifying Large Language Models and Knowledge Graphs: A Roadmap

Shirui Pan, Senior Member, IEEE,
Linhao Luo, Yufei Wang, Chen Chen, Jiapu Wang, Xindong Wu, Fellow, IEEE

Presented by Jixiang Xiong

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Background

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Large Language Models (LLMs)

Most LLMs derive from the Transformer design, which contains the encoder and decoder modules empowered by a self-attention mechanism.

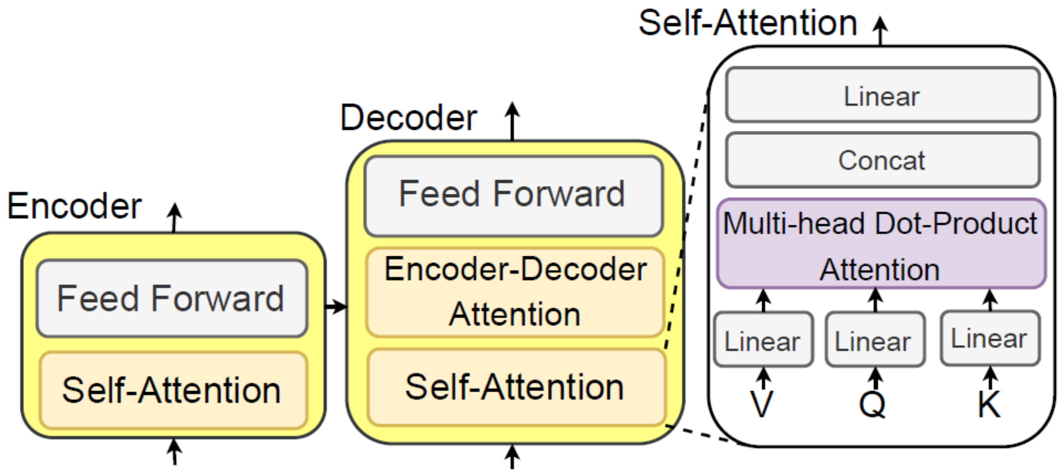


Fig. 3. An illustration of the Transformer-based LLMs with self-attention mechanism.

Large Language Models (LLMs)

- **Encoder-only LLMs**

Training paradigm: predict the mask words in an input sentence

Downstream tasks: text classification and named entity recognition

Examples: BERT, ALBERT, RoBERTa, ELECTRA

- **Encoder-decoder LLMs**

Training paradigm: flexiable

Downstream tasks: summariaztion, translation, and question answering

Examples: GLM-130B, T5, UL2, ST-MoE

- **Decoder-only LLMs**

Training paradigm: predict the next word in the sentence

Examples: Chat-GPT, GPT-4

Large Language Models (LLMs)

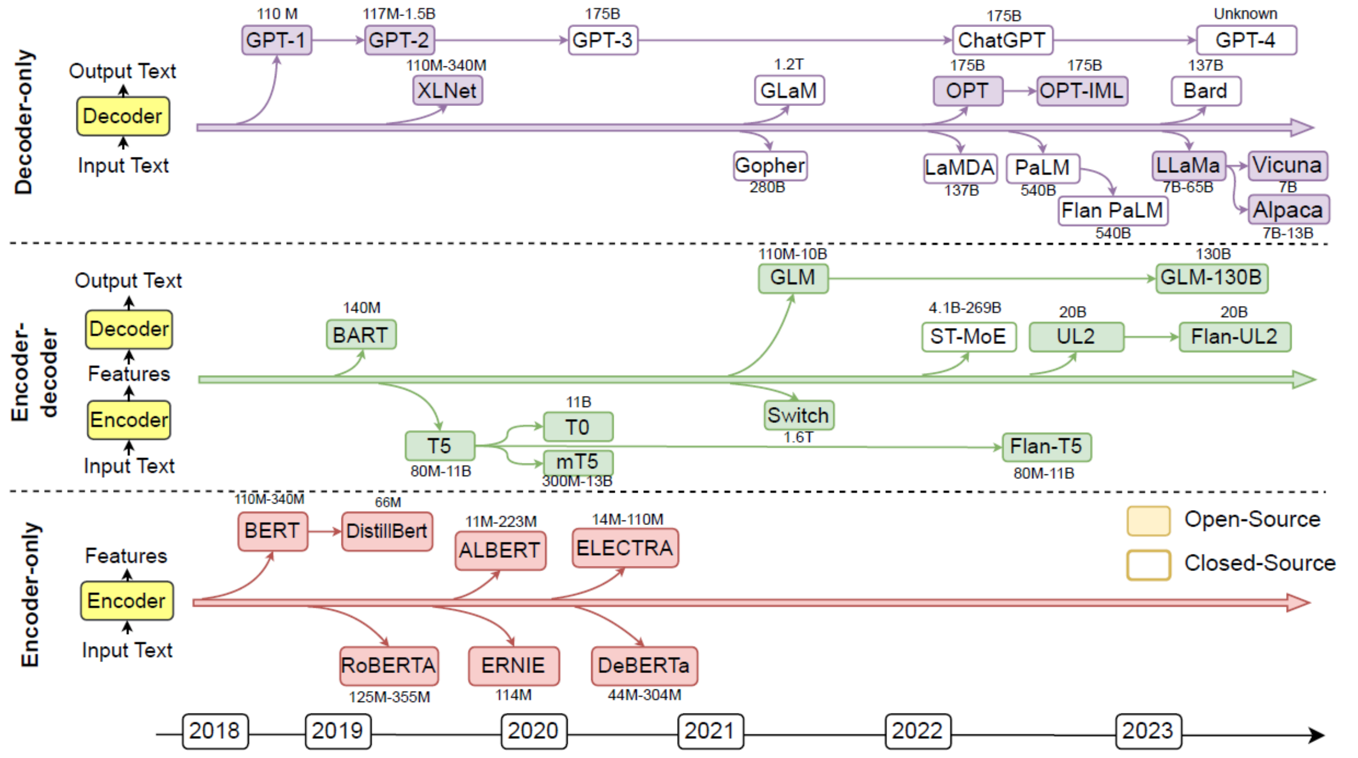


Fig. 2. Representative large language models (LLMs) in recent years. Open-source models are represented by solid squares, while closed source models are represented by hollow squares.

Knowledge Graphs (KGs)

Knowledge graphs (KGs) store structured knowledge as a collection of triples $KG = \{(h, r, t) \in E \times R \times E\}$, where E and R respectively denote the set of entities and relations.

Knowledge Graphs (KGs)

- **Encyclopedic Knowledge Graphs**

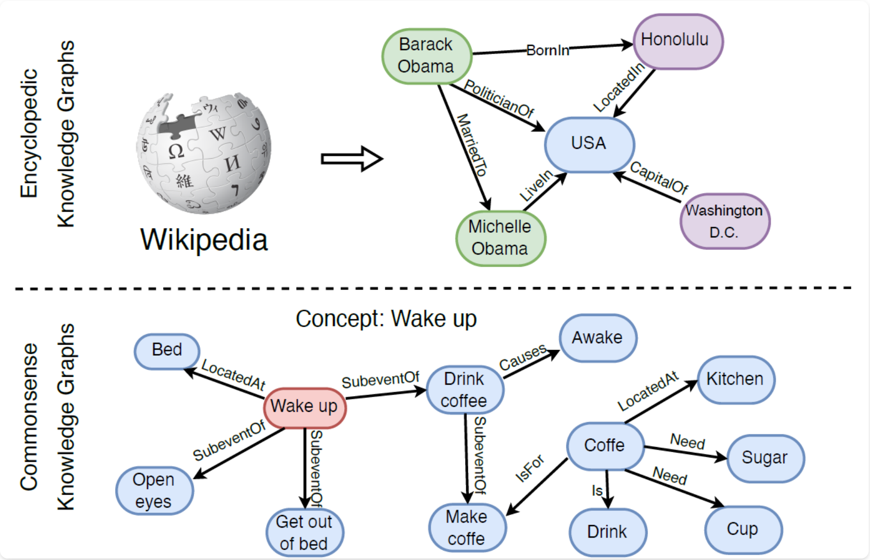
Most ubiquitous KGs, represent the general knowledge in real-world.

Examples: Wikidata, Freebase, Dbpedia, YAGO, NELL, CN-DBpedia, Vikidia, Knowledge Occean

- **Commonsense Knowledge Graphs**

Formulate the knowledge about daily concepts, help computers understand the meanings of words people use.

Examples: ConceptNet, ATOMIC, ASER, TransOMCS, CausalBanK



Knowledge Graphs (KGs)

- **Domain-specific Knowledge Graphs**

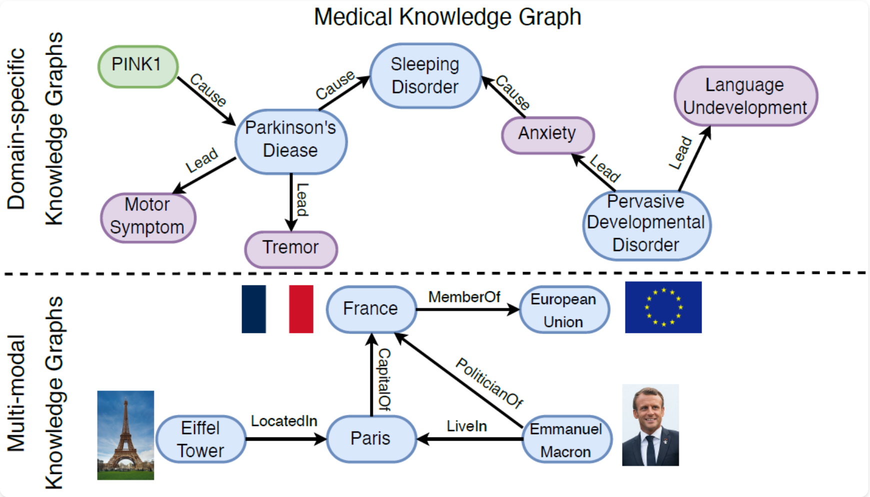
Represent knowledge in a specific domain, e.g., medical, biology, and finance; More accurate and reliable.

Examples: UMLS

- **Multi-modal Knowledge Graphs**

Represent facts in multiple modalities such as images, sounds, and videos.

Examples: IMGpedia, MMKG, Richpedia

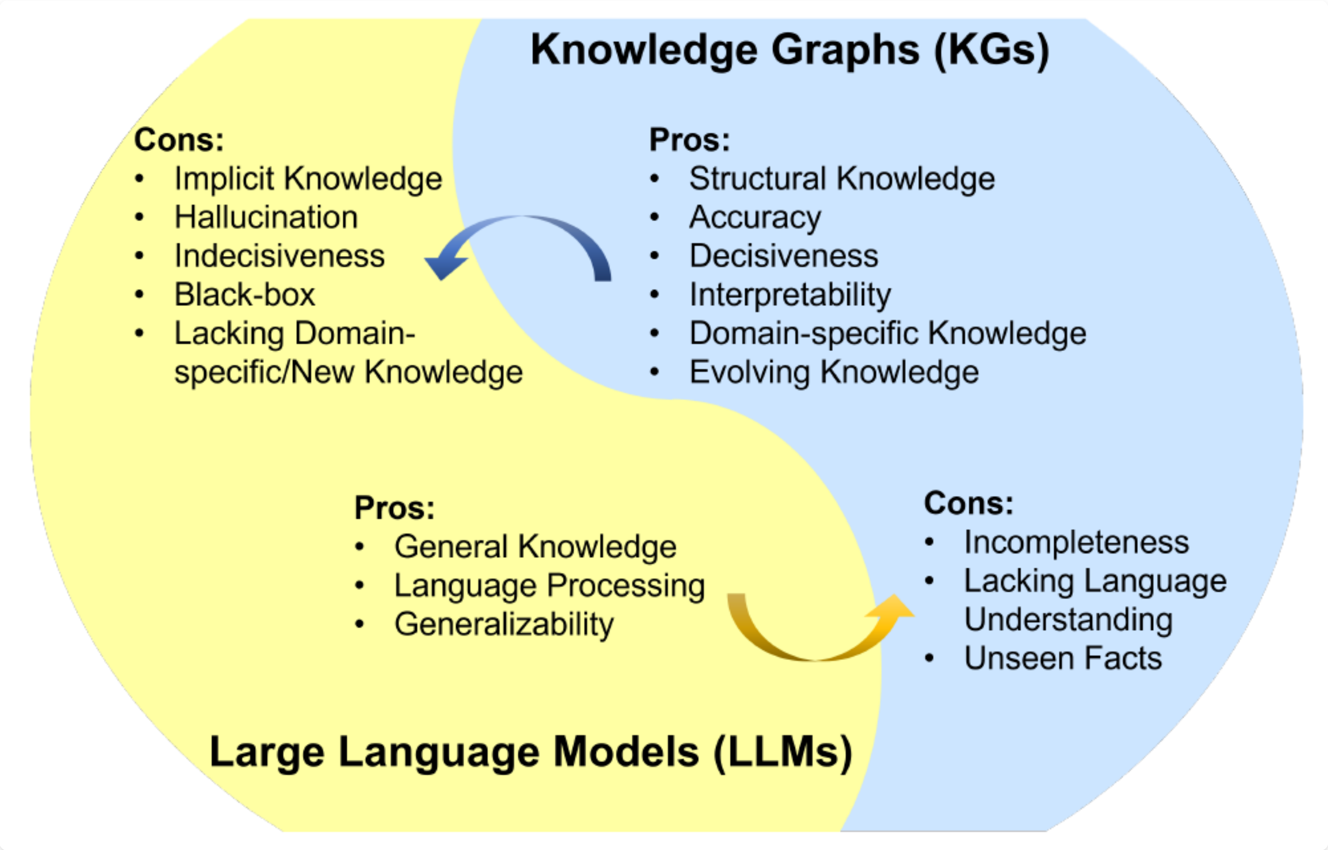


Representative Applications

TABLE 1
Representative applications of using LLMs and KGs.

Name	Category	LLMs	KGs	URL
ChatGPT/GPT-4	Chat Bot	✓		https://shorturl.at/cmsE0
ERNIE 3.0	Chat Bot	✓	✓	https://shorturl.at/sCLV9
Bard	Chat Bot	✓	✓	https://shorturl.at/pDLY6
Firefly	Photo Editing	✓		https://shorturl.at/fkzJV
AutoGPT	AI Assistant	✓		https://shorturl.at/bkoSY
Copilot	Coding Assistant	✓		https://shorturl.at/lKLUV
New Bing	Web Search	✓		https://shorturl.at/bimps
Shop.ai	Recommendation	✓		https://shorturl.at/alCY7
Wikidata	Knowledge Base		✓	https://shorturl.at/lyMY5
KO	Knowledge Base		✓	https://shorturl.at/sx238
OpenBG	Recommendation		✓	https://shorturl.at/pDMV9
Doctor.ai	Health Care Assistant	✓	✓	https://shorturl.at/dhlK0

Pros and Cons



Pros and Cons

Hallucination: generating factually incorrect statements.

Type	Turn	Example
Input-conflicting Hallucination	*User*	Please summarize the following content: My friend Hill and I love playing basketball together. We spend hours on the court, dribbling, shooting, and competing against each other. Our passion for this game brings us closer as good friends.
	Model	Lucas and I love playing basketball and this makes us good friends.
Context-conflicting Hallucination	*User*	Tell me something about the NBA Commissioner.
	Model	In the world's most popular basketball league, the NBA, Commissioner Adam Silver has long been regarded as a leader and decision-maker. Firstly, Silver has claimed his dedication to maintaining fairness and competitiveness in the game. Secondly, Silver has repeatedly emphasized his concern for player health and well-being. In this case, Stern's words and actions clash with his stated goal of caring for player welfare.
Fact-conflicting Hallucination	*User*	Who was the mother of Afonso II, the third king of Portugal?
	Model	The mother of Afonso II was Queen Urraca of Castile.

Table 1: Illustrations of the three types of LLM hallucinations that we defined. For input-conflicting hallucination, the LLM makes a mistake in the person name (*Hill*⇒*Lucas*) during summarizing. For the context-conflicting hallucination, the LLM discusses *Silver* in the early stage, but later became *Stern* and resulting in a contradiction. For the fact-conflicting hallucination, LLMs said the mother of Afonso II was *Queen Urraca of Castile*, while the correct answer is *Dulce Berenguer of Barcelona*.

Arxiv: Siren's Song in the AI Ocean: A Survey on Hallucination in Large Language Models

Roadmap & Categorization

1. Roadmap
2. Categorization

Roadmap

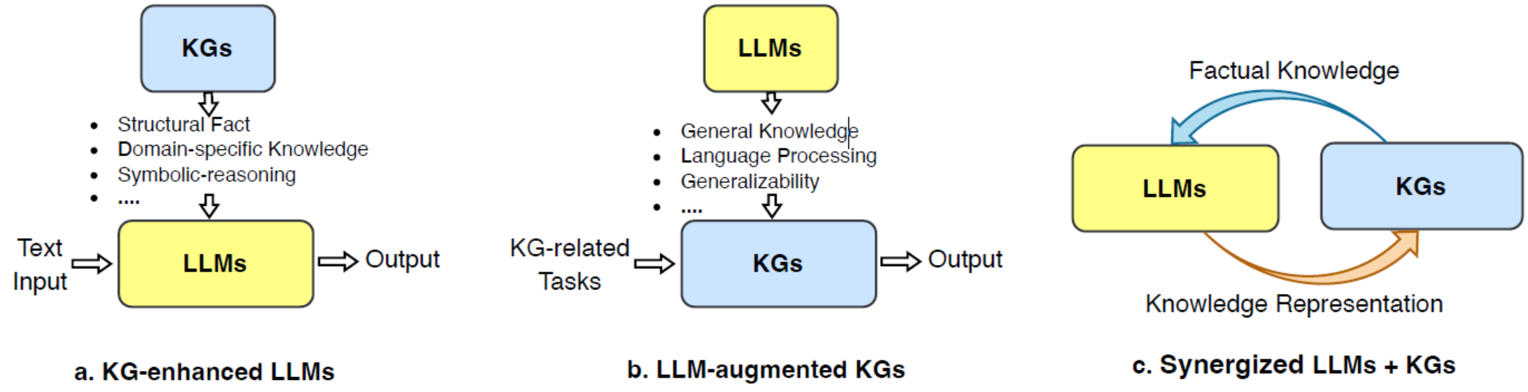
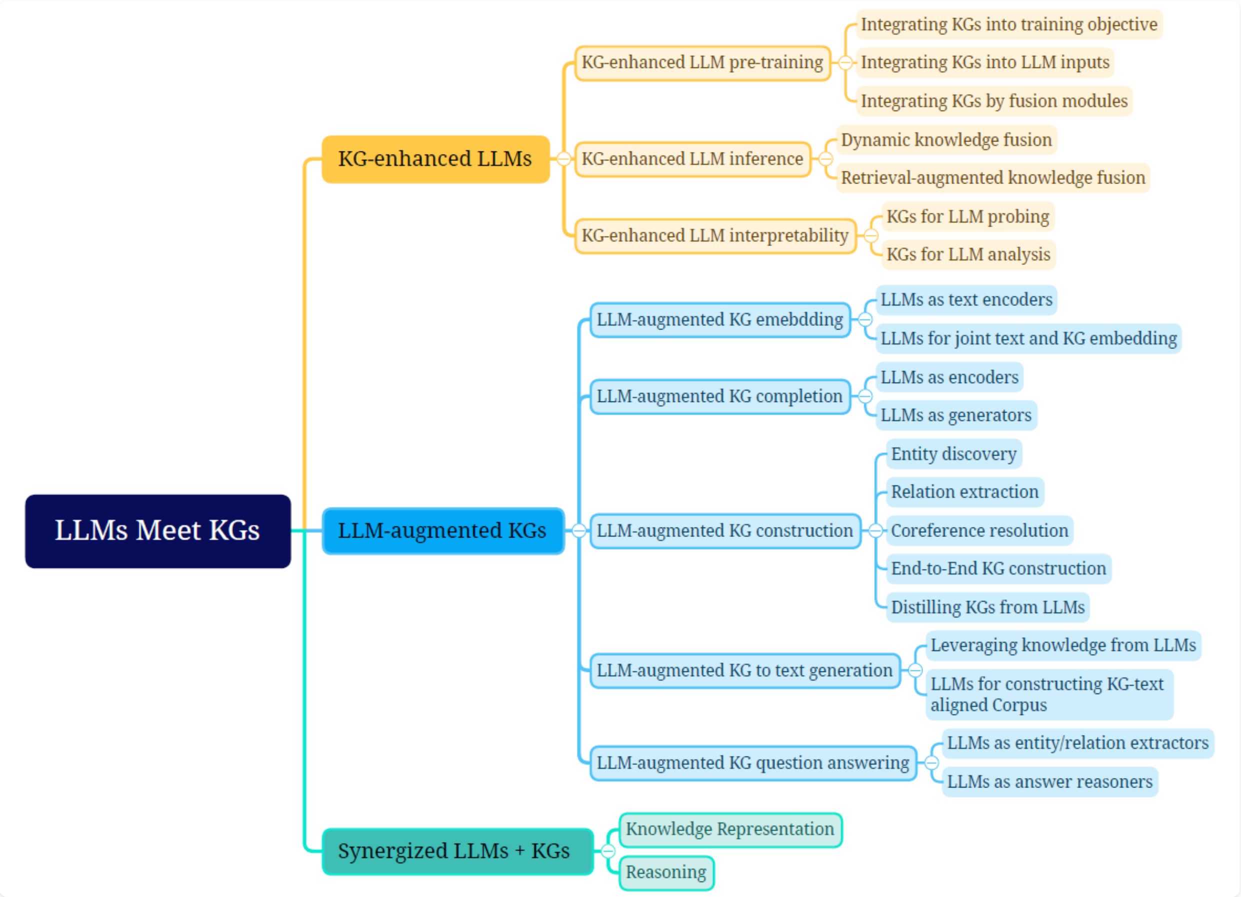


Fig. 6. The general roadmap of unifying KGs and LLMs. (a.) KG-enhanced LLMs. (b.) LLM-augmented KGs. (c.) Synergized LLMs + KGs.

Categorization



KG-enhanced LLMs

1. KG-enhanced LLM Pre-training
2. KG-enhanced LLM Inference
3. KG-enhanced LLM Interpretability

KG-enhanced LLMs

Task	Method	Year	Technique
KG-enhanced LLM pre-training	ERNIE [35]	2019	Integrating KGs into Training Objective
	Skep [103]	2020	Integrating KGs into Training Objective
	GLM [104]	2020	Integrating KGs into Training Objective
	Ebert [105]	2020	Integrating KGs into Training Objective
	KEPLER [40]	2021	Integrating KGs into Training Objective
	Deterministic LLM [106]	2022	Integrating KGs into Training Objective
	KALA [107]	2022	Integrating KGs into Training Objective
	WKLM [108]	2020	Integrating KGs into Training Objective
	K-BERT [36]	2020	Integrating KGs into Language Model Inputs
	CoLAKE [109]	2020	Integrating KGs into Language Model Inputs
	ERNIE3.0 [102]	2021	Integrating KGs into Language Model Inputs
	DkLLM [110]	2022	Integrating KGs into Language Model Inputs
	Dict-BERT [111]	2022	Integrating KGs into Language Model Inputs
	BERT-MK [112]	2020	Integrating KGs into Additional Fusion Modules
	Jaket [113]	2020	Integrating KGs into Additional Fusion Modules
	K-Adapter [114]	2020	Integrating KGs into Additional Fusion Modules
	cokebert [115]	2021	Integrating KGs into Additional Fusion Modules
KG-enhanced LLM inference	QA-GNN [116]	2021	Dynamic Knowledge Fusion
	Jointlk [117]	2022	Dynamic Knowledge Fusion
	GreaseLM [118]	2022	Dynamic Knowledge Fusion
	KGLM [119]	2019	Retrival-augmented knowledge fusion
	REALM [120]	2020	Retrival-augmented knowledge fusion
	RAG [93]	2020	Retrival-augmented knowledge fusion
	Story-fragments [121]	2021	Retrival-augmented knowledge fusion
	EMAT [122]	2022	Retrival-augmented knowledge fusion
KG-enhanced LLM interpretability	LAMA [14]	2019	KGs for LLM probing
	LPAQA [123]	2020	KGs for LLM probing
	Autoprompt [124]	2020	KGs for LLM probing
	Adolphs et al. [125]	2021	KGs for LLM probing
	MedLAMA [126]	2022	KGs for LLM probing
	Alex et al. [127]	2022	KGs for LLM probing
	KagNet [38]	2019	KGs for LLM analysis
	interpret-lm [128]	2021	KGs for LLM analysis
	knowledge-neurons [39]	2021	KGs for LLM analysis
	Shaobo et al. [129]	2022	KGs for LLM analysis

KG-enhanced LLM Pre-training

- **Integrating KGs into Training Objective**
  - Approach 1: give higher masking probability to important entities
  - Approach 2: concat input text with entities in the text as the input

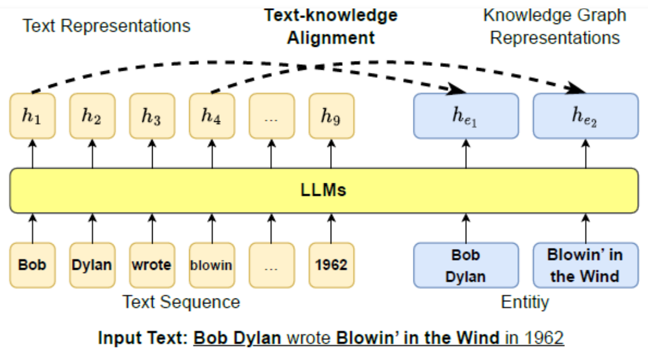


Fig. 9. Injecting KG information into LLMs training objective via text-knowledge alignment loss, where h denotes the hidden representation generated by LLMs.

word-entity alignment training objective

KG-enhanced LLM Pre-training

- **Integrating KGs into LLM Inputs**

Introduce relevant knowledge sub-graph into the inputs of LLMs.

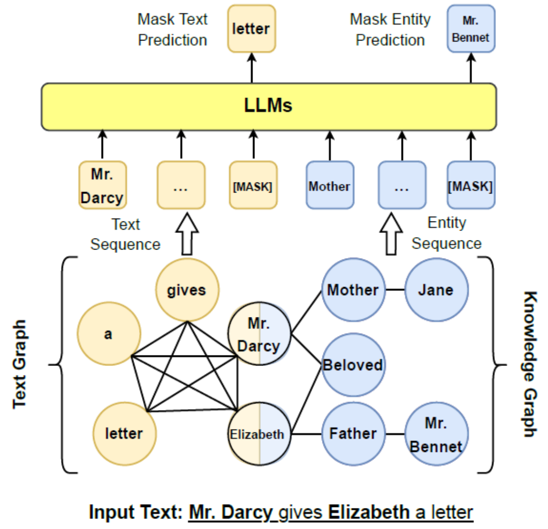


Fig. 10. Injecting KG information into LLMs inputs using graph structure.

KG-enhanced LLM Pre-training

- **Integrating KGs by Additional Fusion Modules**

Separately process the information from KGs and fuse them into LLMs.

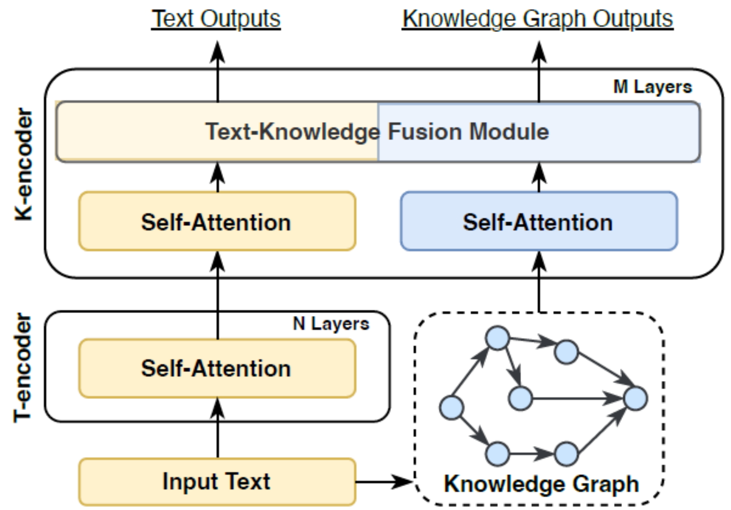


Fig. 11. Integrating KGs into LLMs by additional fusion modules.

KG-enhanced LLM Inference

- **Dynamic Knowledge Fusion**

Leverage a two-tower architecture where one separated module processes the text inputs and the other one processes the relevant knowledge graph inputs. Then, joint them together.

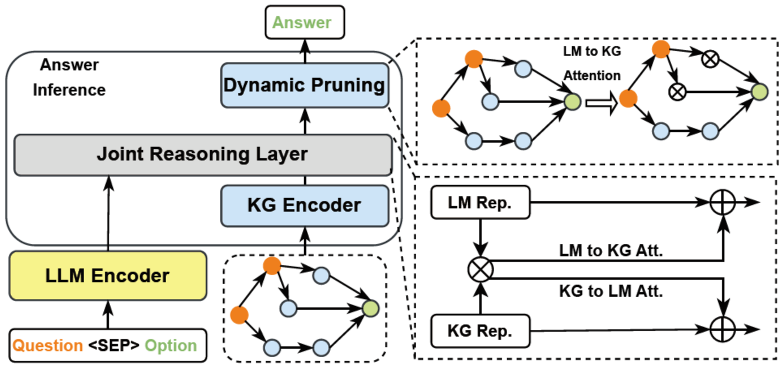


Fig. 12. Dynamic knowledge graph fusion for LLM inference.

KG-enhanced LLM Inference

- **Retrieval-Augmented Knowledge Fusion**

Combine non-parametric and parametric modules to handle the external knowledge.

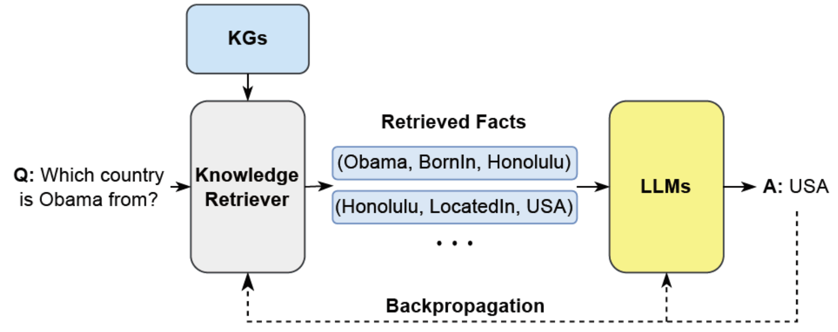


Fig. 13. Retrieving external knowledge to enhance the LLM generation.

KG-enhanced LLM Interpretability

- **KGs for LLM Probing**

Converts the facts in KGs into cloze statements by a predefined prompt template and then use LLMs to predict the missing entity. The prediction results are used to evaluate the knowledge stored in LLMs.

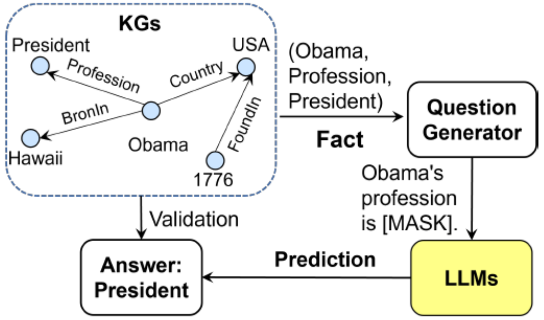


Fig. 14. The general framework of using knowledge graph for language model probing.

KG-enhanced LLM Interpretability

- **KGs for LLM Analysis**

Explain the reasoning process of LLMs by extracting the graph structure from KGs.

Results: LLMs generate the missing factual more by the positionally closed words rather than the knowledge-dependent words.

Claim: LLMs are inadequate to memorize factual knowledge because of the inaccurate dependence.

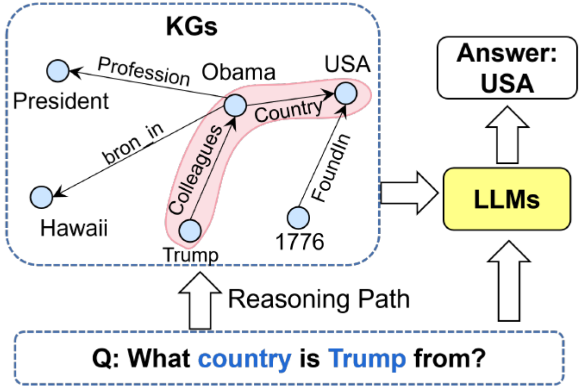


Fig. 15. The general framework of using knowledge graph for language model analysis.

LLM-augmented KGs

1. LLM-augmented KG Embedding
2. LLM-augmented KG Completion
3. LLM-augmented KG Construction
4. LLM-augmented KG-to-text Generation
5. LLM-augmented KG Question Answering

LLM-augmented KG Embedding

- **LLMs as Text Encoders**

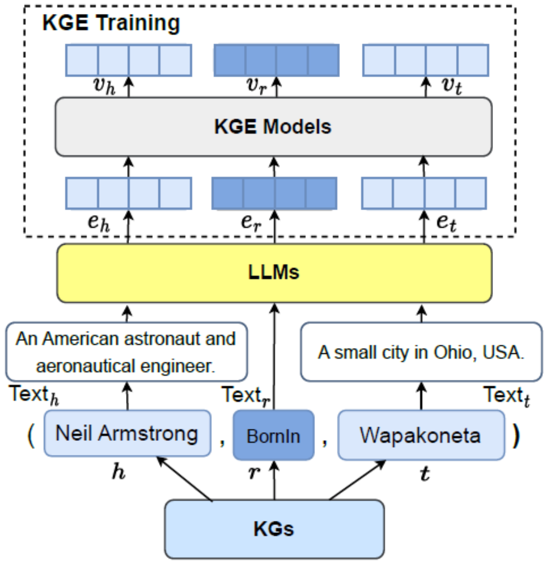


Fig. 16. LLMs as text encoder for knowledge graph embedding (KGE).

- **LLMs for Joint Text and KG Embedding**

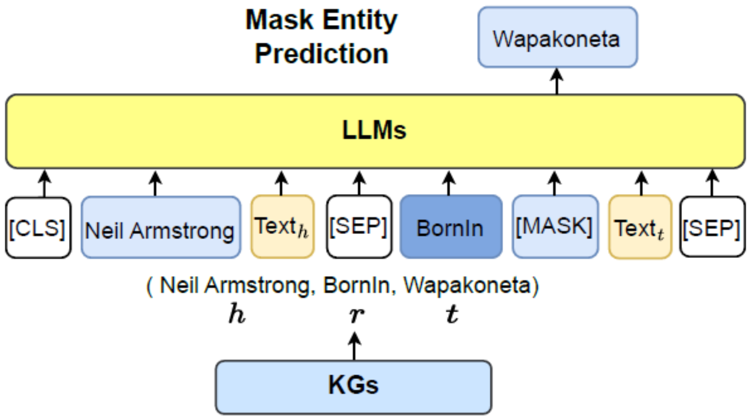


Fig. 17. LLMs for joint text and knowledge graph embedding.

LLM-augmented KG Completion

- **LLM as Encoders (PaE)**

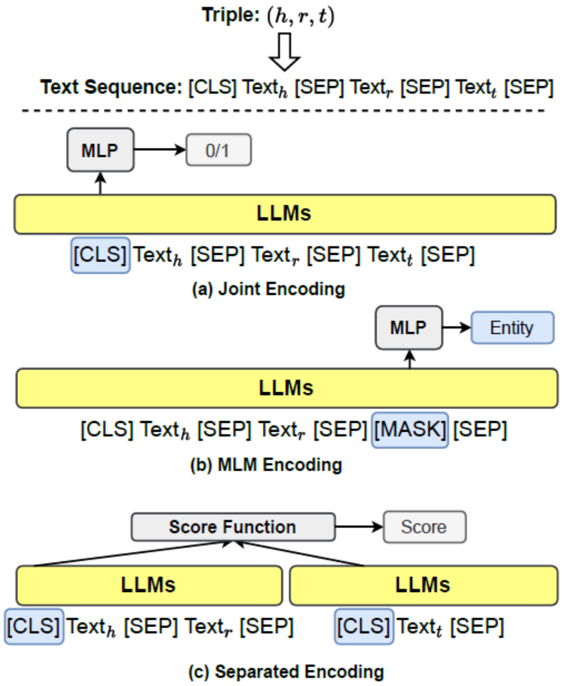


Fig. 18. The general framework of adopting LLMs as encoders (PaE) for KG Completion.

- **LLM as Generators (PaG)**

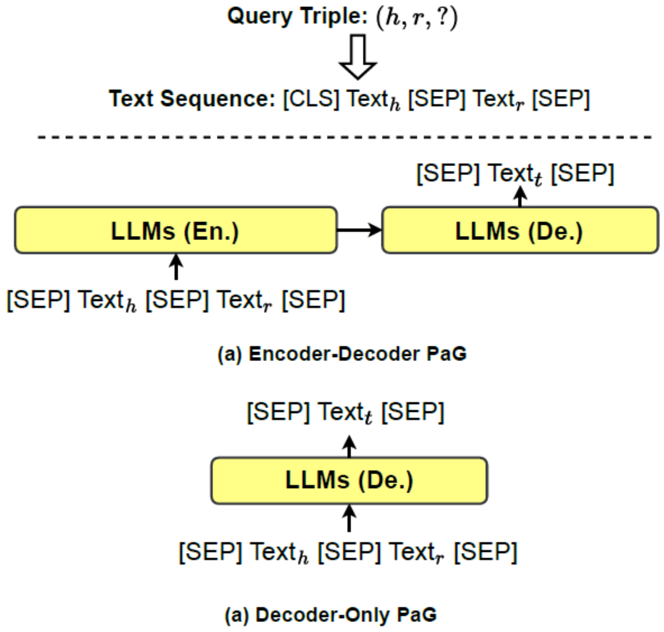


Fig. 19. The general framework of adopting LLMs as decoders (PaG) for KG Completion. The En. and De. denote the encoder and decoder, respectively.

LLM-augmented KG Construction

- **End-to-End KG Construction**

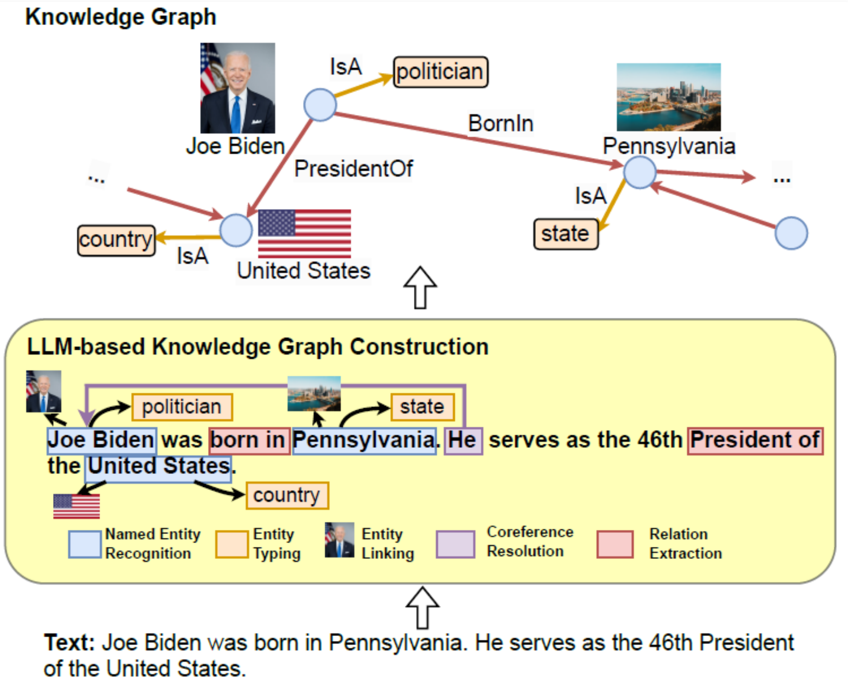


Fig. 21. The general framework of LLM-based KG construction.

- **Distilling Knowledge Graphs from LLMs**

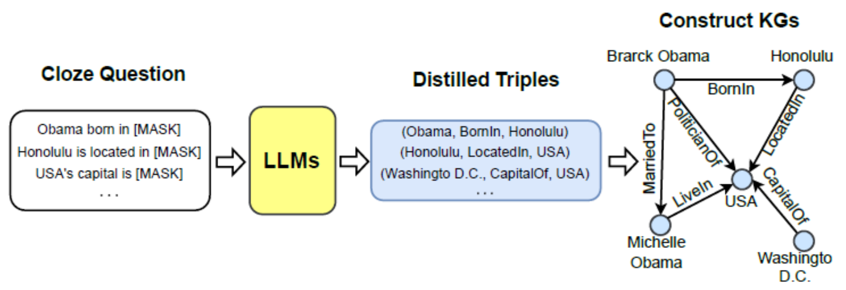


Fig. 22. The general framework of distilling KGs from LLMs.

LLM-augmented KG-to-text Generation

- **Leveraging Knowledge from LLMs**

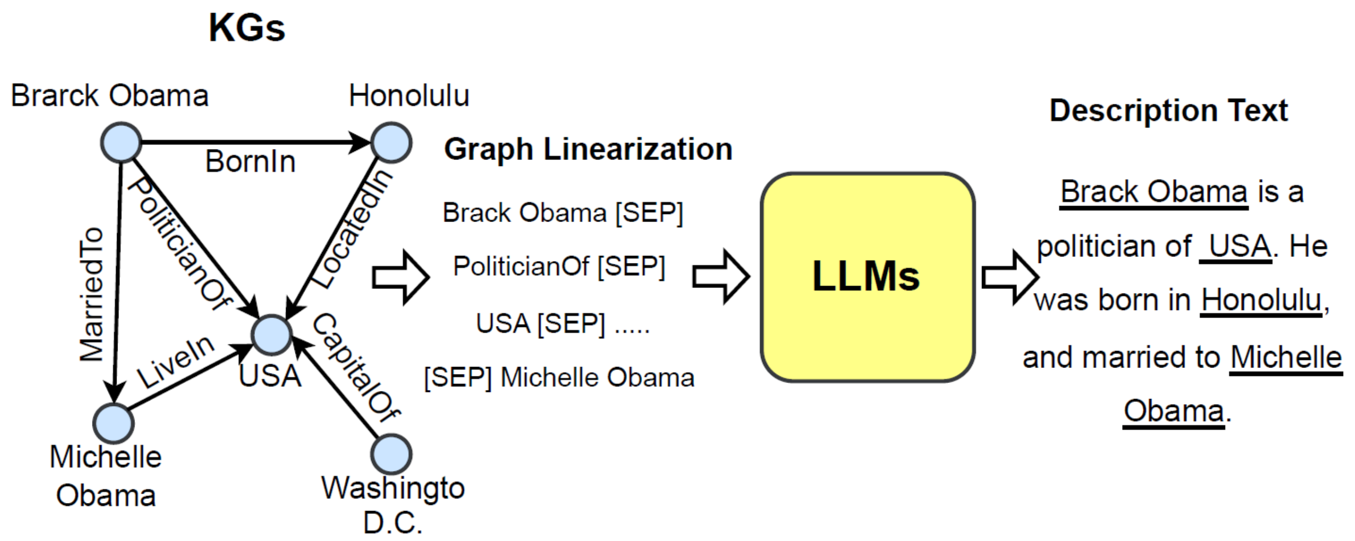


Fig. 23. The general framework of KG-to-text generation.

LLM-augmented KG Question Answering

- LLMs as entity/relation extractors
- LLMs as answer reasoners

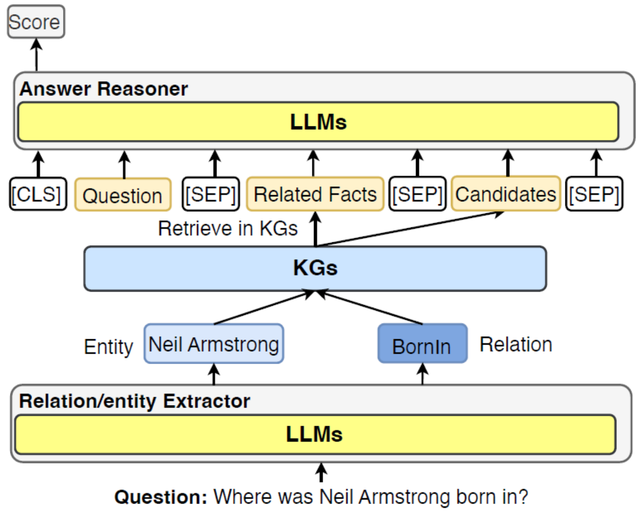


Fig. 24. The general framework of applying LLMs for knowledge graph question answering (KGQA).

Synergized LLMS + KGS

1. Knowledge Representation
2. Reasoning

Knowledge Representation

The knowledge in the text corpus is usually implicit and unstructured, while the knowledge in KGs is explicit and structured.

It is necessary to align the knowledge in the text corpus and KGs to represent them in a unified way.

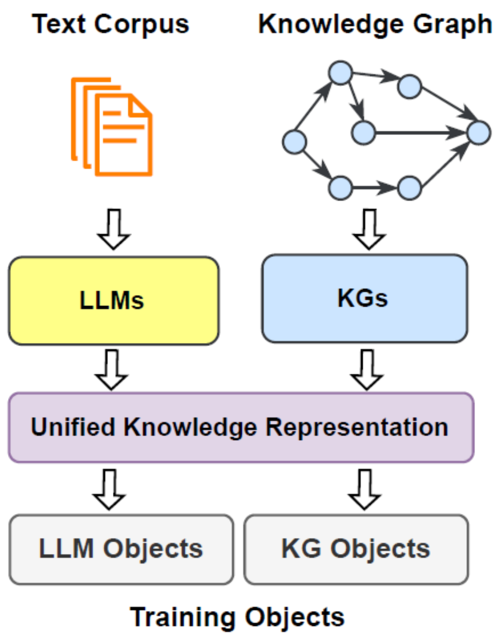


Fig. 25. The general framework of unifying LLMs and KGs for knowledge representation.

Reasoning

- Question answering task: utilize LLMs to process the text question and guide the reasoning step on the KGs.
- Knowledge graph reasoning task: transform the conventional logical rules into a language sequence and then ask LLMs to reason the final outputs.
- Adopt LLMs to generate the logical query, which is executed on the KGs to obtain structural context. Last, the structural context is fused with textual information to generate the final output.

Future Directions

- **KGs for Hallucination Detection in LLMs**
- **KGs for Editing Knowledge in LLMs**
- **KGs for Black-box LLMs Knowledge Injection**
- **Multi-Modal LLMs for KGs**
- **LLMs for Understanding KG Structure**
- **Synergized LLMs and KGs for Birectional Reasoning**

Thanks