KG-FIT: Knowledge Graph Fine-Tuning Upon Open-World Knowledge

Pengcheng Jiang, Lang Cao, Cao Xiao, Parminder Bhatia, Jimeng Sun, and Jiawei Han

University of Illinois at Urbana Champaign, GE HealthCare

NEURAL INFORMATION PROCESSING SYSTEMS

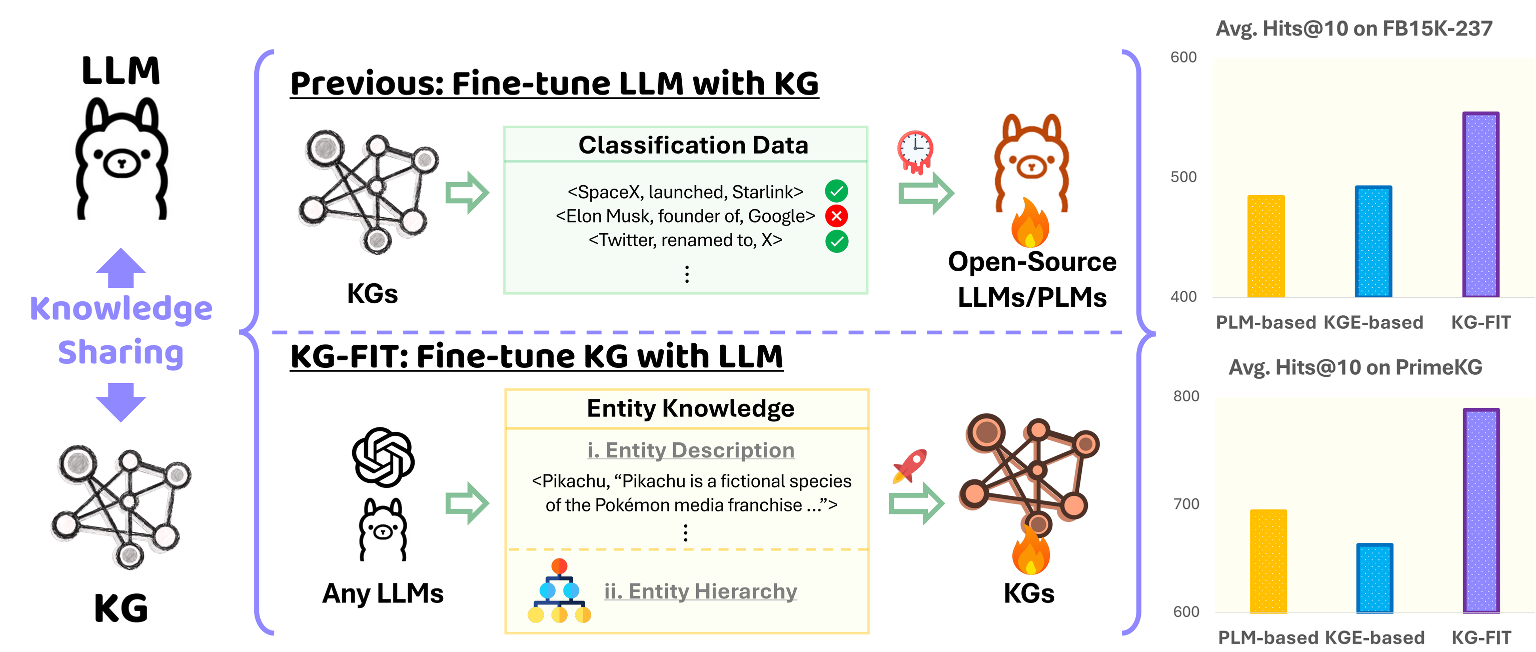
Introduction

Current Challenges:

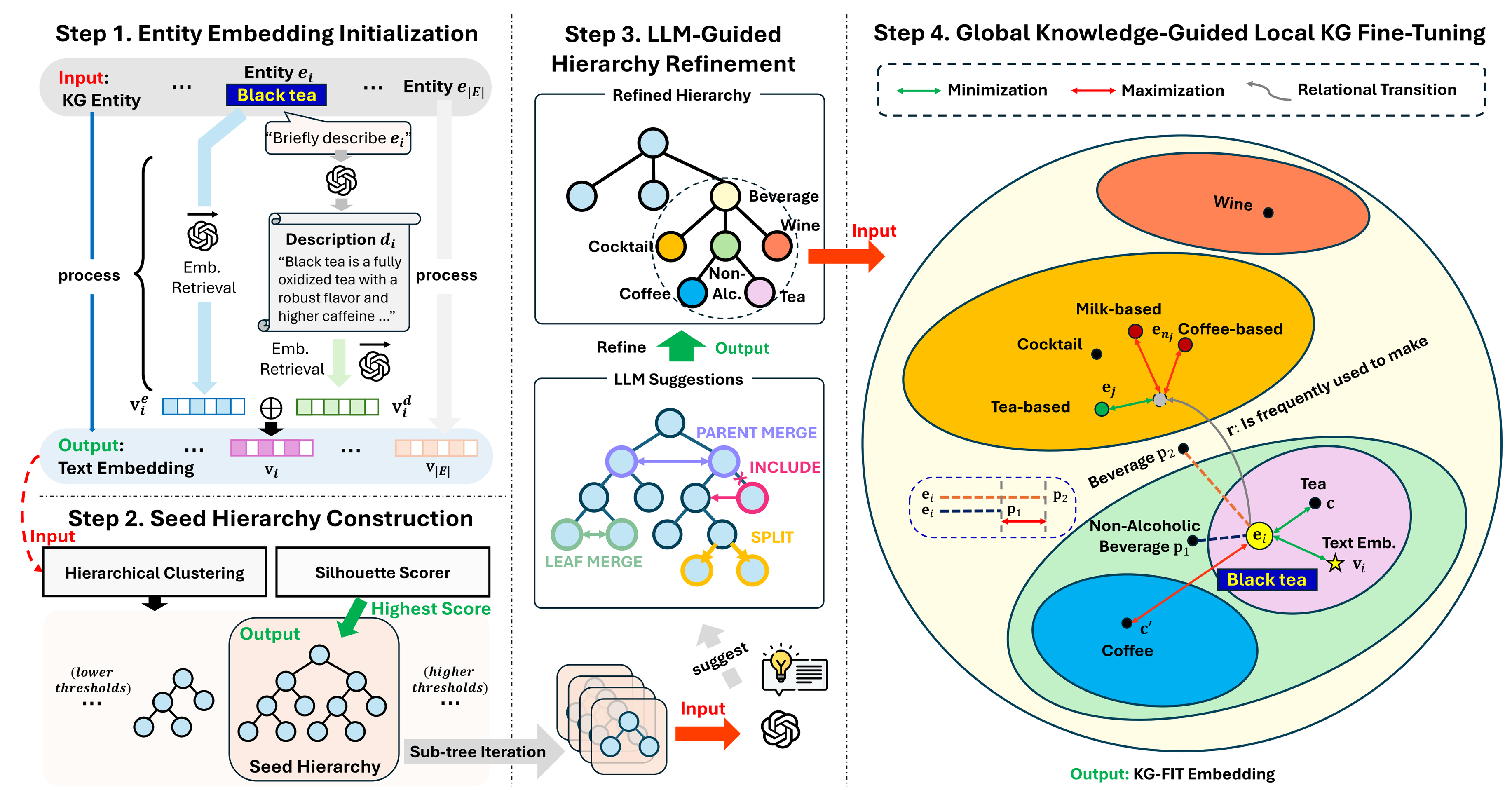
- Knowledge Graph Embeddings are crucial for AI systems but often limited to structure alone
- Existing methods that combine KGs with language models face key limitations:
  - High computational costs during training and inference
  - Limited ability to leverage extensive knowledge in modern LLMs
  - Difficulty keeping up with rapidly evolving generative LLMs

Our Solution: KG-FIT

- A novel framework that directly incorporates knowledge from LLMs into KG embeddings
- Key innovations:
  - LLM-guided hierarchical structure construction
  - Effective integration of global semantics from LLMs with local semantics from KGs
  - No need to fine-tune the language models themselves



Our Method: KG-FIT



KG-FIT framework includes the following steps:

Step 1: Entity Embedding Initialization
Create initial entity embeddings by concatenating:

- Entity name embedding
- Entity description (generated by LLM) embedding

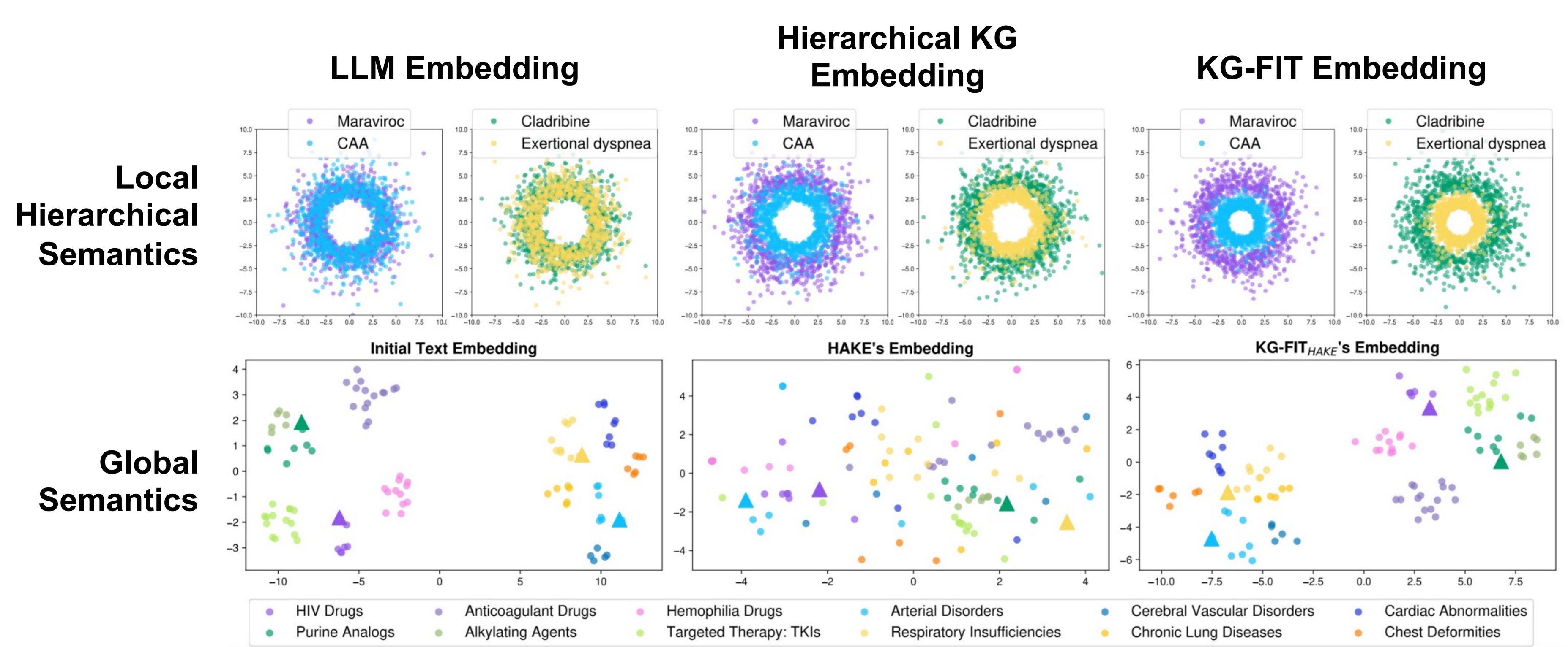
Step 2: Seed Hierarchy Construction
Apply agglomerative clustering to entity embeddings
Select optimal hierarchy using silhouette score

Step 3: LLM-Guided Hierarchy Refinement
Refine the seed hierarchy constructed with LLM's suggestions through an iterative bottom-up tree editing process

Step 4: Knowledge Graph Fine-Tuning

1. Initialize entity and relation embeddings
2. Fine-tune the KG embedding with score functions (defined any base KGE models) and the knowledge in the entity hierarchy.

Embedding Comparison



Our KG-FIT embedding captures both local and global semantics.
In this example, KG-FIT can accurately predict:
Local: (1) Maraviroc has drug effect on coronary artery atherosclerosis (CAA), (2) Cladribine has drug effect of exertional dyspnea
Global: (1) Maraviroc is a type of HIV drugs, (2) Cladribine is a type of Purine Analog.

Performance Comparison

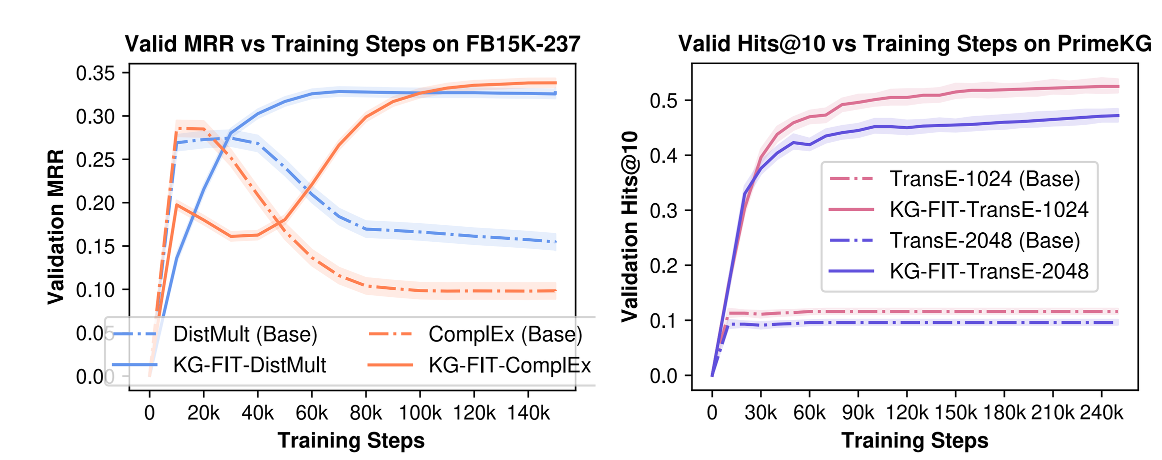
		FB15K-237					YAGO3-10					PrimeKG				
PLM-based Embedding Methods																
Model	PLM	MR	MRR	H@1	H@5	H@10	MR	MRR	H@1	H@5	H@10	MR	MRR	H@1	H@5	H@10
KG-BERT [22]*	BERT	153	.245	.158	–	.420	–	–	–	–	–	–	–	–	–	–
StAR [23]*	RoBERTa	**117**	.296	.205	–	.482	–	–	–	–	–	–	–	–	–	–
PKGC [28]	RoBERTa	184	.342	.236	.441	.525	1225	.501	.426	.596	.660	219	.485	.391	.565	.625
C-LMKE [26]*	BERT	141	.306	.218	–	.484	–	–	–	–	–	–	–	–	–	–
KGT5 [25]*	T5	–	.276	.210	–	.414	–	.426	.368	–	.528	–	–	–	–	–
KG-S2S [24]*	T5	–	.336	.257	–	.498	–	–	–	–	–	–	–	–	–	–
SimKGC [27]	BERT	–	.336	.249	–	.511	–	–	–	–	–	168	.527	.524	.679	.742
CSProm-KG [32]	BERT	–	.358	.269	–	.538	1145	.488	.451	.624	.675	157	.540	.492	.652	.745
LLM Emb. (zero-shot)	TE-3-S	2044	.023	.002	.035	.068	22741	.009	.000	.016	.024	5581	.000	.000	.000	.000
	TE-3-L	1818	.030	.004	.048	.085	18780	.015	.000	.019	.032	4297	.001	.000	.000	.000

			FB15K-237					YAGO3-10					PrimeKG				
Structure-based Embedding Methods																	
Model	Frame	$\mathcal{H}$	MR	MRR	H@1	H@5	H@10	MR	MRR	H@1	H@5	H@10	MR	MRR	H@1	H@5	H@10
TransE	Base [14]	—	233	.287	.192	.389	.478	1250	.500	.398	.626	.685	182	.048	.000	.043	.124
	KG-FIT	Seed	142	.345	.242	.457	.547	952	.520	.429	.638	.700	80	.298	.000	.315	.516
		LHR	122	**.362**	.264	.478	.568	**529**	.544	.463	.650	.705	69	.334	.000	.342	.536
• • •																	
pRotatE	Base[19]	—	188	.310	.205	.399	.502	974	.477	.385	.573	.655	118	.491	.399	.593	.681
	KG-FIT	Seed	160	.355	.257	.461	.558	910	.525	.436	.622	.693	75	.635	.538	.745	.809
		LHR	**119**	**.371**	**.277**	**.483**	**.572**	829	**.550**	.464	.648	**.710**	69	**.649**	**.574**	**.779**	**.833**
RotatE	Base [19]	—	190	.333	.241	.428	.528	1620	.495	.402	.550	.670	57	.539	.447	.646	.727
	KG-FIT	Seed	141	.354	.261	.464	.555	790	.529	.440	.643	.708	**46**	.622	.517	.740	.805
		LHR	**120**	**.369**	**.274**	**.488**	**.570**	**744**	**.563**	**.475**	**.658**	**.722**	**34**	.645	.532	.758	.817
HAKE	Base [20]	—	184	.344	.247	.435	.538	1220	530	.431	.634	.681	95	.595	.515	.708	.760
	KG-FIT	Seed	162	.358	.268	.470	.563	854	.541	.455	.647	.703	82	.638	.540	.747	.808
		LHR	137	**.362**	**.275**	**.485**	**.572**	**810**	**.568**	**.474**	**.662**	**.718**	**42**	**.682**	**.605**	**.785**	**.835**

Key Findings:
(1) KG-FIT significantly outperforms SOTA PLM- and structure-based methods
(2) Performance gain by LHR (LLM-guided hierarchy refinement) is huge

- Suggesting the importance of high-quality hierarchical knowledge of entities

Training Insights



Key Findings:
(1) KG-FIT effectively addresses both overfitting (LHS)and underfitting (RHS) challenges of KGE training
(2) Hierarchical structure provides natural regularization
(3) Integration of LLM knowledge helps reach better convergence points

Paper Code

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