A Graph Perspective to Probe Structural Patterns of Knowledge in LLMs

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Knowledge Intelligence for Discovery and Decision-making (KIND) Lab

• LLMs as neural KBs but graph structure overlooked; • Introduce triplet & entity knowledgeability; • Reveal knowledge homophily among neighboring nodes; • Apply GNN to predict entity knowledge; • Fine-tune on low-knowledge triplets for better performance.

Triplet Knowledgeability

Prompt 1: LLM-based Triplet Evaluation

System Message: Evaluate the statement based on your knowledge and respond with `True` or `False`.

Given: Triplet $\mathcal{T} = (sub,\ rel,\ obj)$.

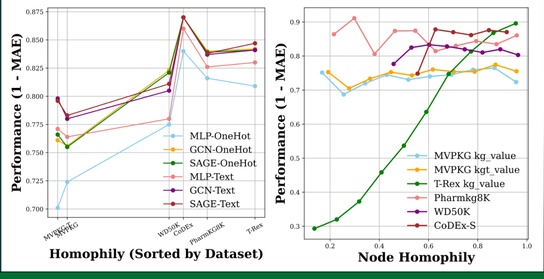
Relational Template Map: $T:\ rel \mapsto$ "$\{sub\}\ \ldots\ \{obj\}$".

Procedure:

1. Retrieve relation-based template $t = T(relation)$.
2. Instantiate statement $S = t[\{sub\} \to sub,\ \{obj\} \to obj]$.
3. Prompt **System Msg + User Msg:** S to the LLM.
4. Return "True" or "False."

Entity Knowledge Score Regression with GNNs

Model	T-Rex	WD50K	Pharm	MVPKG(w/o t)	CoDEx
N-MLP	81%	78%	82%	72% (70%)	84%
N-GCN	84%	**82%**	**84%**	76% (76%)	87%
N-SAGE	84%	82%	84%	76% (77%)	**87%**
T-MLP	83%	78%	83%	76% (77%)	86%
T-GCN	84%	81%	84%	78% (**80%**)	87%
T-SAGE	**84%**	81%	84%	**78%** (79%)	87%



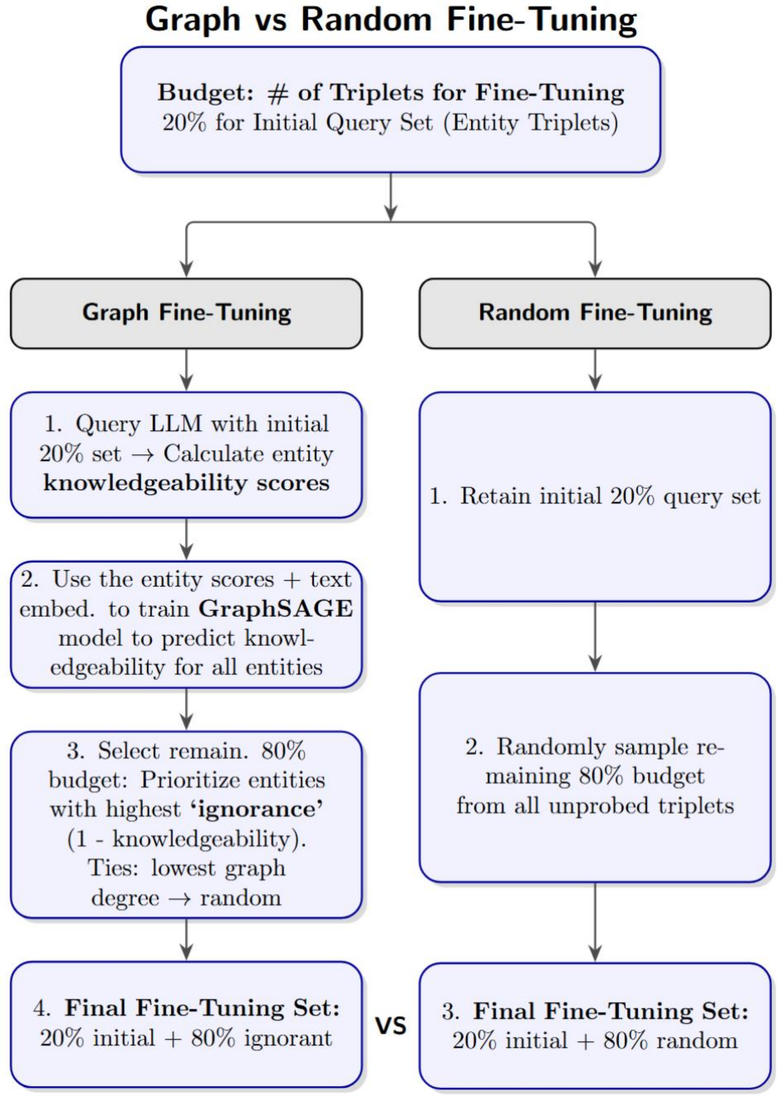
Entity Knowledgeability and Homophily

$$\mathcal{K}(v_i) = |\mathcal{T}(v_i)|^{-1} \sum_{(v_i, r_{ij}, v_j) \in \mathcal{T}(v_i)} \mathcal{K}(v_i, r_{ij}, v_j)$$

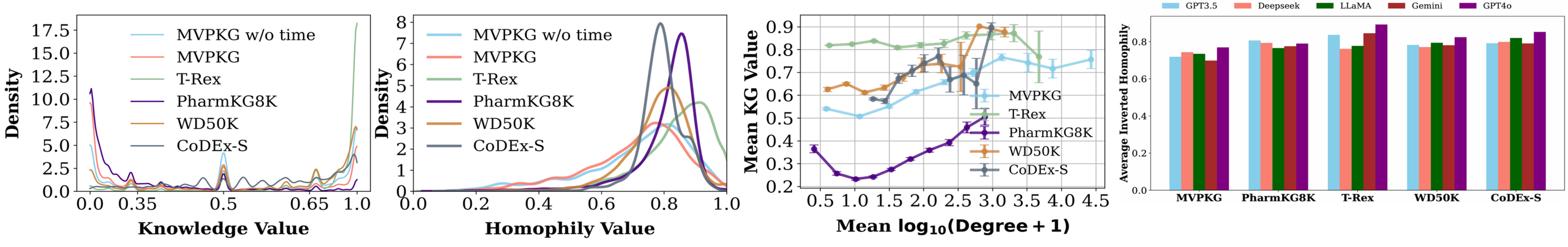
$$\mathcal{H}_{v_i} = 1 - \frac{1}{|\mathcal{N}(v_i)|} \sum_{v_j \in \mathcal{N}(v_i)} |\mathcal{K}(v_i) - \mathcal{K}(v_j)|$$

Graph vs Random FT Performance

Dataset	Model	Base	Random-FT	Graph-FT
T-Rex	Llama3 8B	63.25	86.40	**89.05**
	Mistral 7B	63.95	81.85	**91.90**
	Qwen2.5 7B	56.05	**84.80**	83.25
Pharm	Llama3 8B	17.80	34.85	**36.95**
	Mistral 7B	55.30	41.30	**60.70**
	Qwen2.5 7B	39.50	70.20	**74.40**
WD50	Llama3 8B	54.75	57.75	**58.75**
	Mistral 7B	42.87	**56.25**	55.12
	Qwen2.5 7B	49.37	63.00	**64.75**
MVPKG w/o t	Llama3 8B	26.10	30.70	**44.50**
	Mistral 7B	52.30	65.10	**76.70**
	Qwen2.5 7B	37.60	41.30	**65.10**
CoDEx	Llama3 8B	64.87	**78.75**	75.62
	Mistral 7B	58.50	72.12	**88.00**
	Qwen2.5 7B	62.37	67.00	**70.87**
Average Performance		49.64	62.09	**69.04**



Analysis of Structural Patterns



(a) **(b)** **(c)** **(d)**

Distribution of node **(a)** knowledgeability and **(b)** homophily for each dataset; **(c)** Node knowledgeability increases as node degree increase; **(d)** Average homophily for all datasets given by different LLMs exceeds 0.6