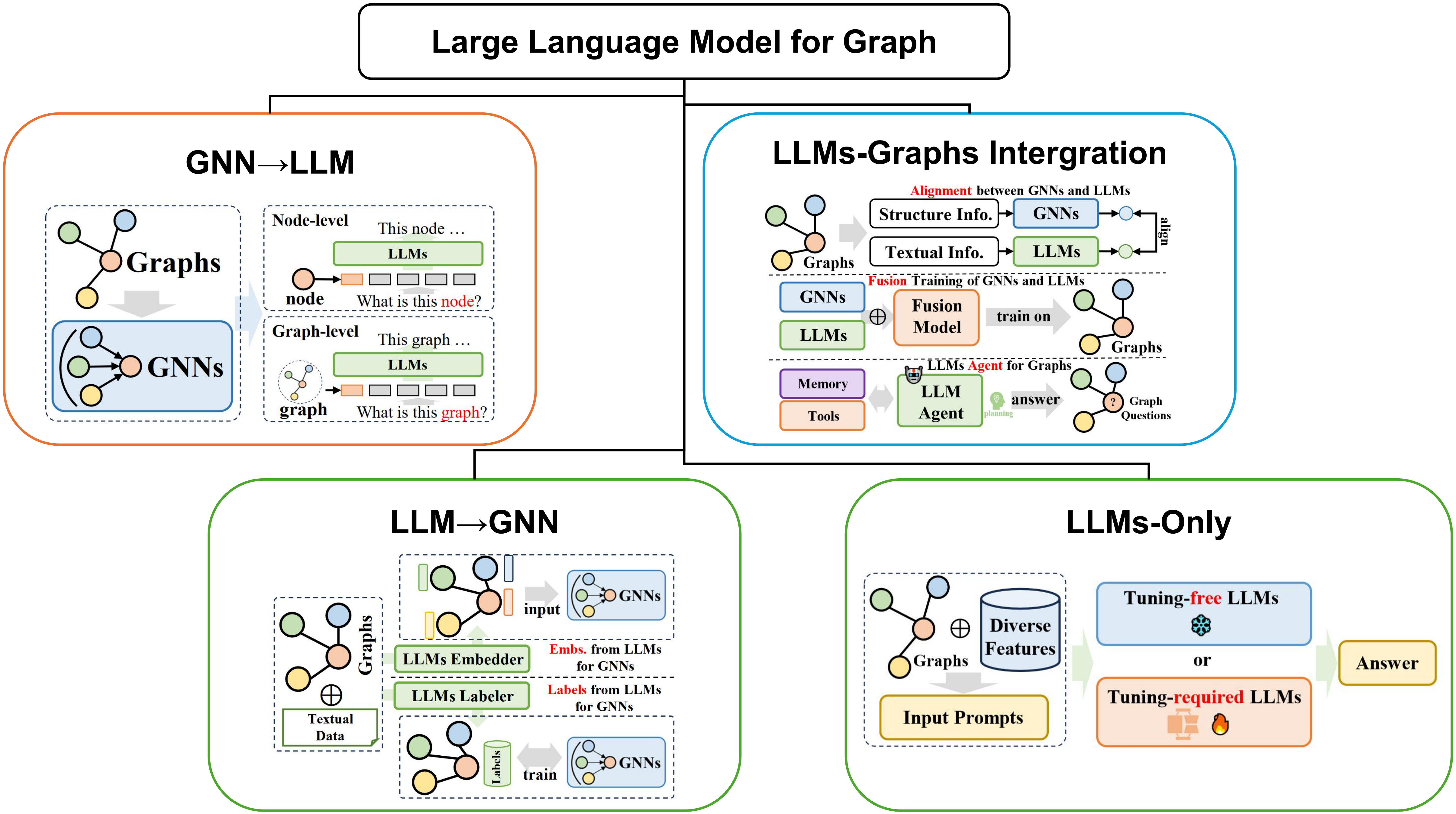
中国科学院信息工程研究所
INSTITUTE OF INFORMATION ENGINEERING,CAS

ASCII

图与大模型

南艺璇 2024/09/14



A Survey of Large Language Models for Graphs, KDD 2024

Outline

一、LLMs-Only

a) Tuning-free

b) Tuning-required

- ZeroG: Investigating Cross-dataset Zero-shot Transferability in Graphs, KDD 2024

二、GNN→LLM

a) Node-level

- GraphTranslator: Aligning Graph Model to Large Language Model for Open-ended Tasks, WWW 2024

b) Graph-level

- Graph Neural Prompting with Large Language Models, AAAI 2024

三、LLM→GNN

a) Labels from LLMs for GNNs

- GraphEdit: Large Language Models for Graph Structure Learning
- Label-free node classification on graphs with large language models, ICLR 2024

四、LLMs-Graphs Intergration

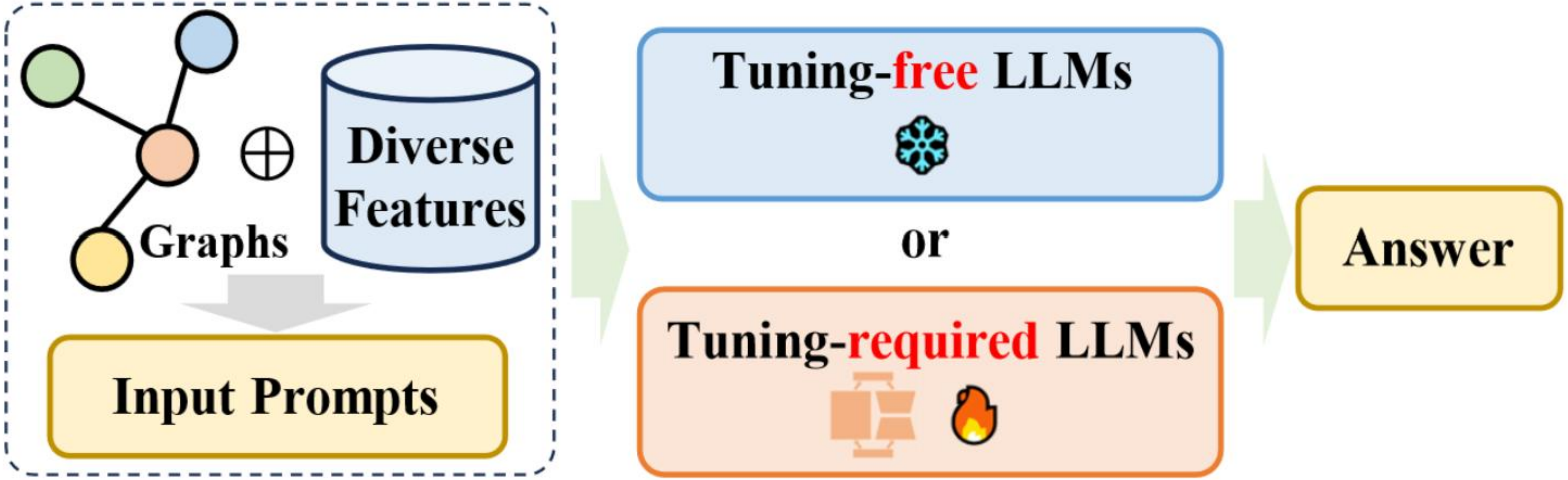
a) Alignment between GNNs and LLMs

- Grenade: Graph-Centric Language Model for Self-Supervised Representation Learning on Text-Attributed Graphs

LLMs-Only

概述

- 为LLM构建适当的提示来获得与图相关的回答。
- 从图结构中设计LLM可以直接理解的Prompt/指令调优LLM对齐图知识。



A Survey of Large Language Models for Graphs, KDD 2024

相关工作

1. **Tuning-free**
2. **Tuning-required**
   - ZeroG: Investigating Cross-dataset Zero-shot Transferability in Graphs, KDD 2024

LLMs-Only　Tuning-free

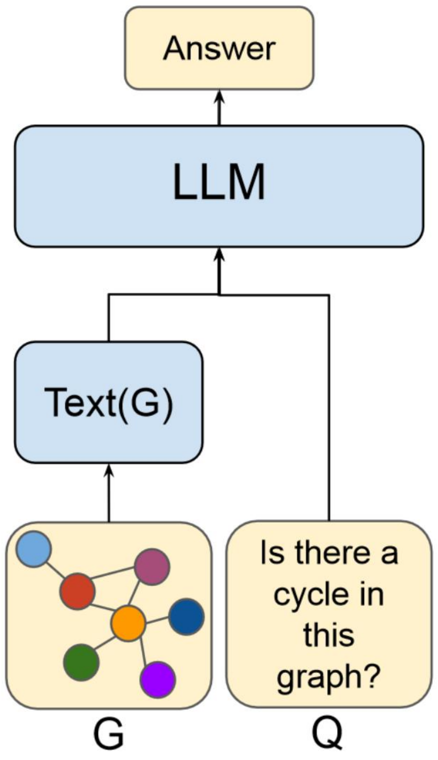
- **Motivation**:

  LLM是否可以将图结构的文本描述映射到基础概念空间并用自然语言解决图算法问题?

- **Experiment Results**:

  LLM具有图推理能力。
  但在面对复杂图推理任务时，没能学习生成中间步骤的正确方法。
  上下文学习中的样本可能让LLM分散注意力。

  不同的图编码方式、图结构、图任务，都会影响LLM的性能。



LLM单独处理图问题的能力可能没那么好

Can language models solve graph problems in natural language?, NIPS 2023
Talk like a Graph: Encoding Graphs for Large Language Models

ZeroG: Investigating Cross-dataset Zero-shot Transferability in Graphs

- **Motivation**：

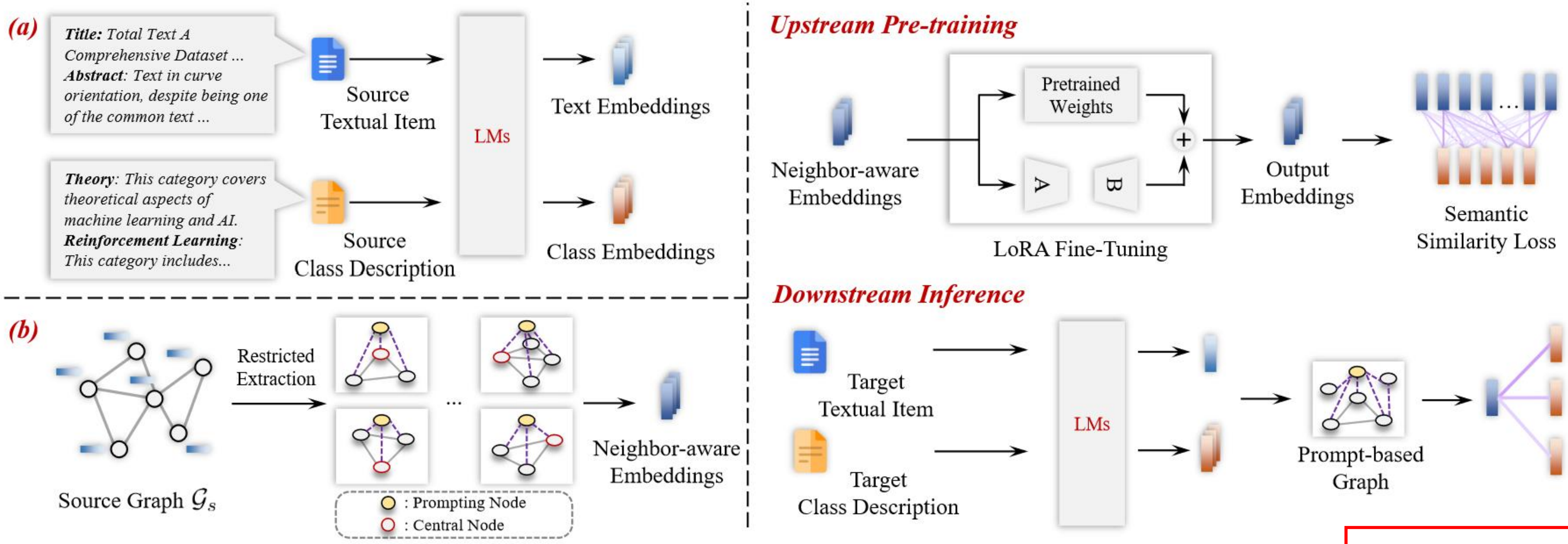
传统 GNN 在零样本迁移方面面临挑战，主要是由于维度未对齐、标签空间不匹配和负迁移的问题。
直接将节点信息输入LLM进行零样本推理，面临数据泄露以及LLM很难融入图结构的问题。

- 维度错位? 用 LM 统一图表示学习，统一映射到语义空间。
- 标签空间不匹配? 在预训练和推理阶段将节点分类任务重新表述为文本相似性任务。
- 负迁移? 引入子图采样，通过提示节点增强一般语义信息。

ZeroG: Investigating Cross-dataset Zero-shot Transferability in Graphs, KDD 2024

LLMs-Only Tuning-required

- **Method**：



Restricted Extraction： 只考虑采样子图种类超过总类一半的子图。

Prompting Node： 连接到子图内所有节点，通过语言模型生成表示。

B.2.1 Cora. The Cora [61] dataset is a fundamental resource in the field of graph learning, particularly within the realm of machine learning research. It represents a network of scientific publications. There are 7 categories in Cora: Theory, covering theoretical aspects of machine learning and AI; Reinforcement Learning, including research on reinforcement learning, a type of machine learning; Genetic Algorithms, dealing with genetic algorithms, a type of optimization algorithm inspired by natural evolution. Neural Networks, focusing on artificial neural networks, a subset of machine learning. Probabilistic Methods, pertaining to research on probabilistic methods in machine learning, using probability mathematics to handle uncertainty and make predictions. Case Based, focusing on case-based reasoning in AI, a method that solves new problems by referring to similar past cases. Rule Learning, involving the generation of rules for decision-making systems. The average degree of Cora is 4.

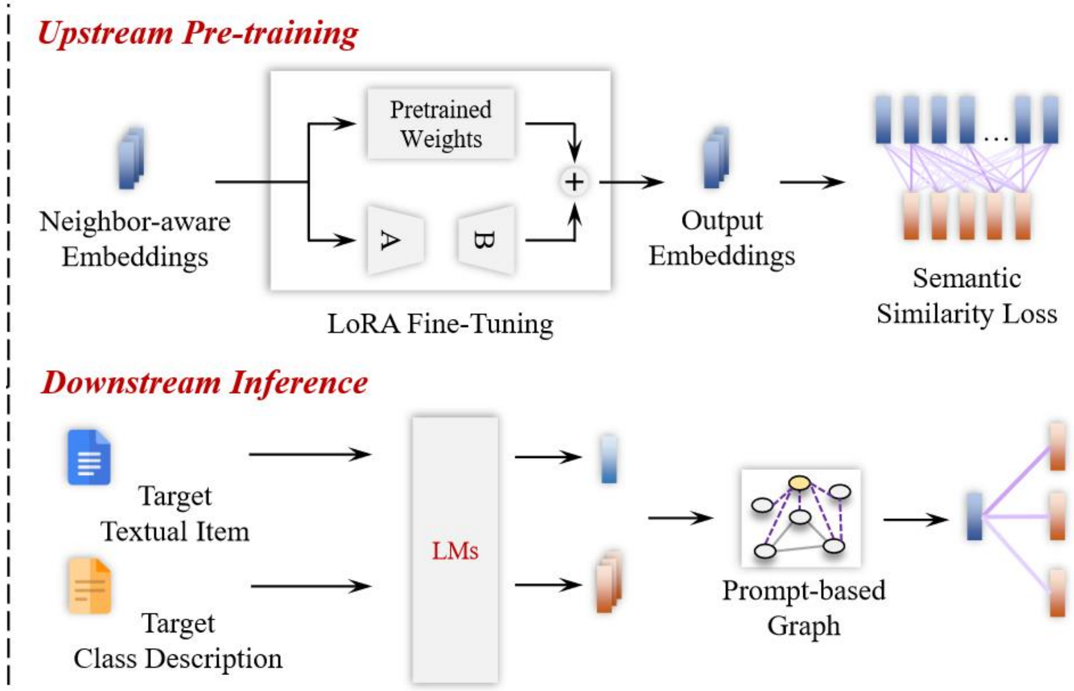
Neighborhood Aggregation：

$$A_{norm} = M^{-\frac{1}{2}} A M^{-\frac{1}{2}} \qquad H^{(t+1)} = A_{norm} H^{(t)}$$

ZeroG: Investigating Cross-dataset Zero-shot Transferability in Graphs, KDD 2024

LLMs-Only Tuning-required

- **Method**：



Upstream Pre-training：

LoRA 微调

Downstream Inference：

用语言模型为数据集生成节点和类嵌入，用提示节点通过邻域聚合更新节点嵌入，最后得到类预测分数。

ZeroG: Investigating Cross-dataset Zero-shot Transferability in Graphs, KDD 2024

LLMs-Only　Tuning-required

- **Experiment**:

域内转移:

Methods	$\mathcal{A}$	$\mathcal{S}$	Cora	Pubmed	Citeseer	P-Home	P-Tech
			zero-shot settings				
DGI [56]	✓	✗	19.97	43.89	21.12	33.06	55.83
GraphCL [63]	✓	✗	26.22	43.73	20.59	37.44	62.63
GraphMAE [19]	✓	✗	34.79	48.23	34.62	37.04	73.37
BERT [12]	✗	✓	19.90	34.79	23.76	37.32	56.44
RoBERTa [34]	✗	✓	28.91	27.33	30.95	35.50	66.31
E5 [58]	✗	✓	39.70	41.93	45.89	57.56	59.17
Sent-BERT [40]	✗	✓	52.25	41.71	47.52	63.22	67.21
OFA [31]	✓	✓	27.07	37.87	37.92	32.86	71.03
ZeroG (ours)	✓	✓	**68.72**	**78.02**	**64.94**	**73.20**	**82.96**
			semi-supervised settings				
GCN* [25]	-	-	81.50	79.00	70.30	73.85	93.28
GAT* [55]	-	-	83.00	79.00	72.50	73.46	88.89

ZeroG: Investigating Cross-dataset Zero-shot Transferability in Graphs, KDD 2024

LLMs-Only Tuning-required

- **Experiment**:

跨域转移:

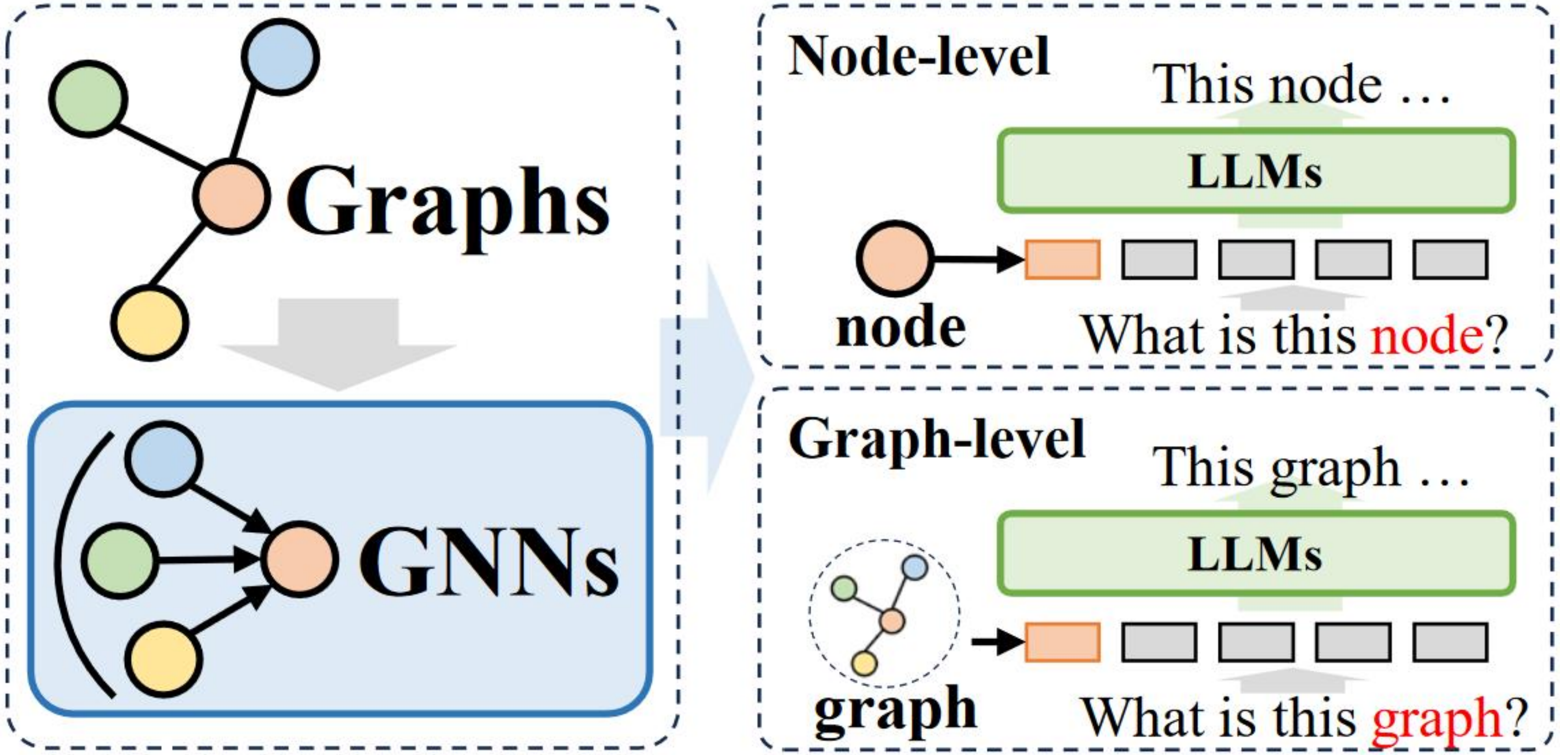
Test	Pre-training	OFA	In-D	ZeroG
Wiki-CS	Arxiv ∪ Cora ∪ Pubmed ∪ Citeseer	48.42	-	53.28
Wiki-CS	P-Home ∪ P-Tech	21.09	-	60.97
Cora	P-Home ∪ P-Tech	18.57	68.72	67.65(-1.07%)
Pubmed	P-Home ∪ P-Tech	31.89	78.02	69.12(-8.90%)
Citeseer	P-Home ∪ P-Tech	20.78	64.94	53.17(-11.77%)
P-Home	Arxiv ∪ Cora ∪ Pubmed ∪ Citeseer	35.73	73.20	71.45(-1.75%)
P-Tech	Arxiv ∪ Cora ∪ Pubmed ∪ Citeseer	62.10	82.96	83.20(+0.24%)

ZeroG: Investigating Cross-dataset Zero-shot Transferability in Graphs, KDD 2024

GNN→LLM

概述

- GNN 作为结构编码器，以增强 LLM 对图结构的理解。
- GNN 将图数据编码为包含结构信息的token序列，然后输入到 LLM 中与自然语言对齐。



A Survey of Large Language Models for Graphs, KDD 2024

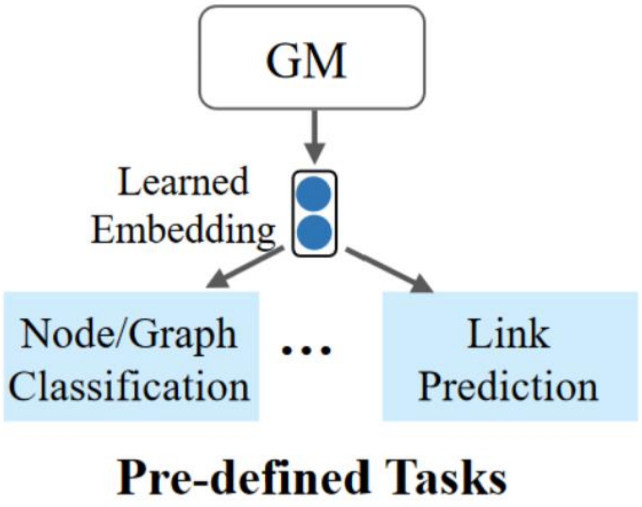
相关工作

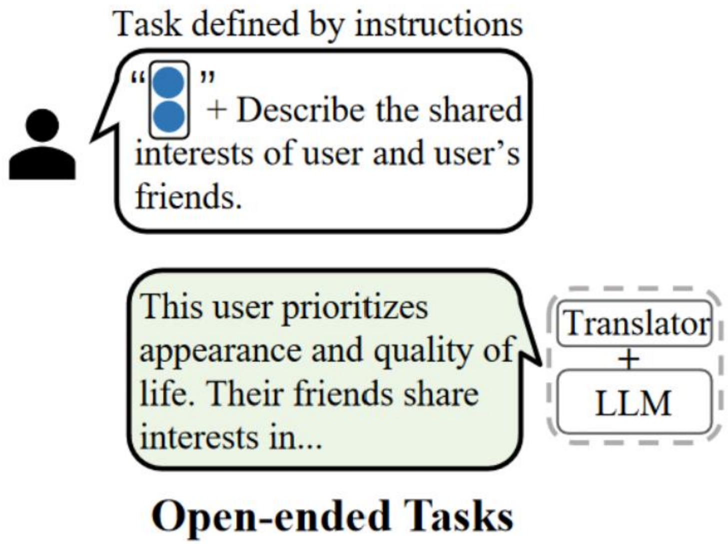
1. **Node-level**
   - GraphTranslator: Aligning Graph Model to Large Language Model for Open-ended Tasks, WWW 2024
2. **Graph-level**
   - Graph Neural Prompting with Large Language Models, AAAI 2024

GraphTranslator: Aligning Graph Model to Large Language Model for Open-ended Tasks

- **Motivation**:

用LLM作为Graph Model的增强器，可以对预定义的任务进行准确的预测，但无法处理**开放式任务**，缺乏交互性和灵活性，可解释性。因此作者希望设计一个既能解决预定义任务又能解决开放式任务的模型。

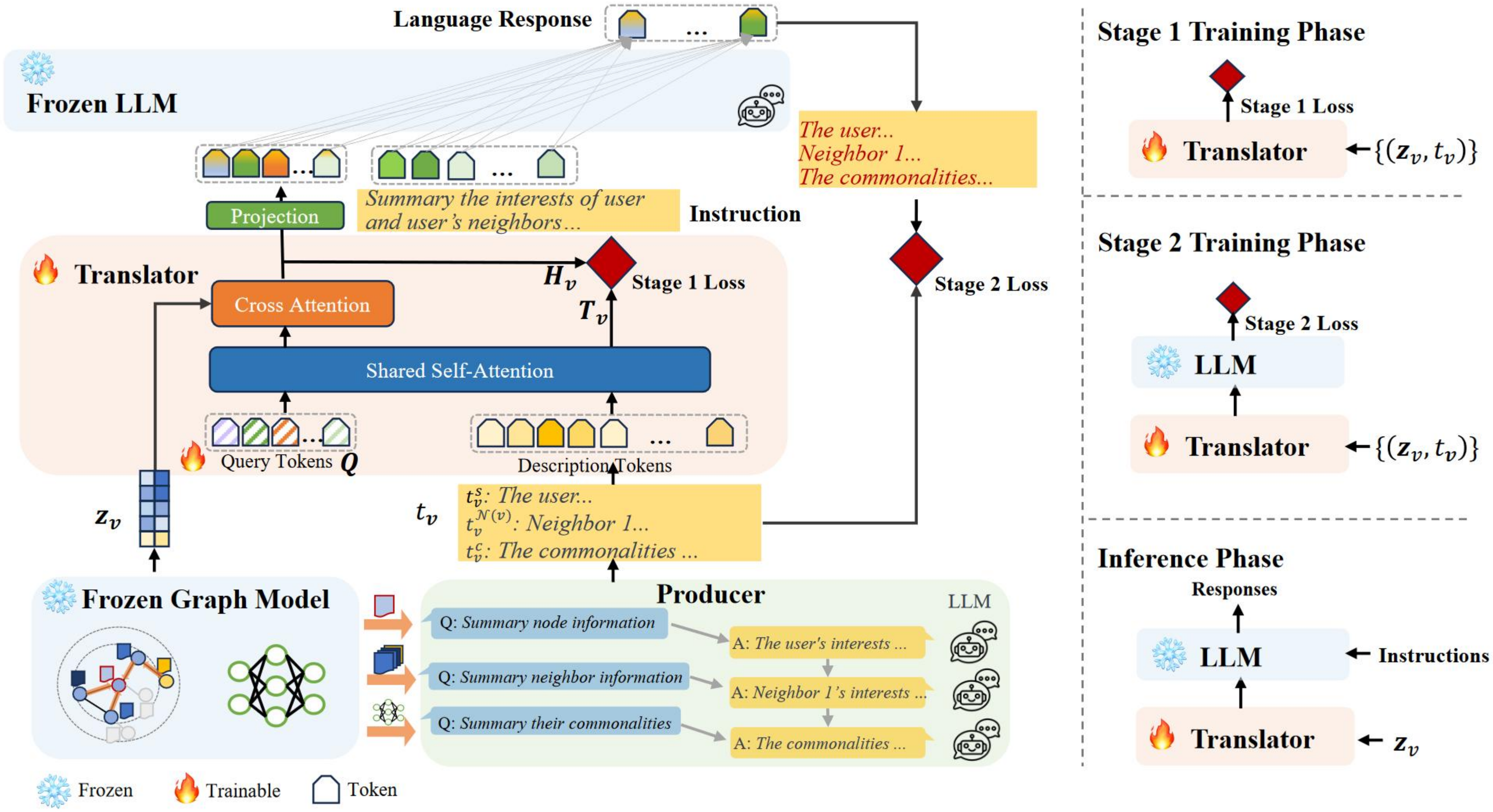




GraphTranslator: Aligning Graph Model to Large Language Model for Open-ended Tasks, WWW 2024

GNN→LLM Node-level

- **Method**



GraphTranslator: Aligning Graph Model to Large Language Model for Open-ended Tasks, WWW 2024

GNN→LLM Node-level

- **Method**

1. Frozen Graph Model & Frozen LLM

GraphSAGE对节点的局部图信息进行编码，生成节点嵌入z_v。

ChatGLM2-6B

2. Producer

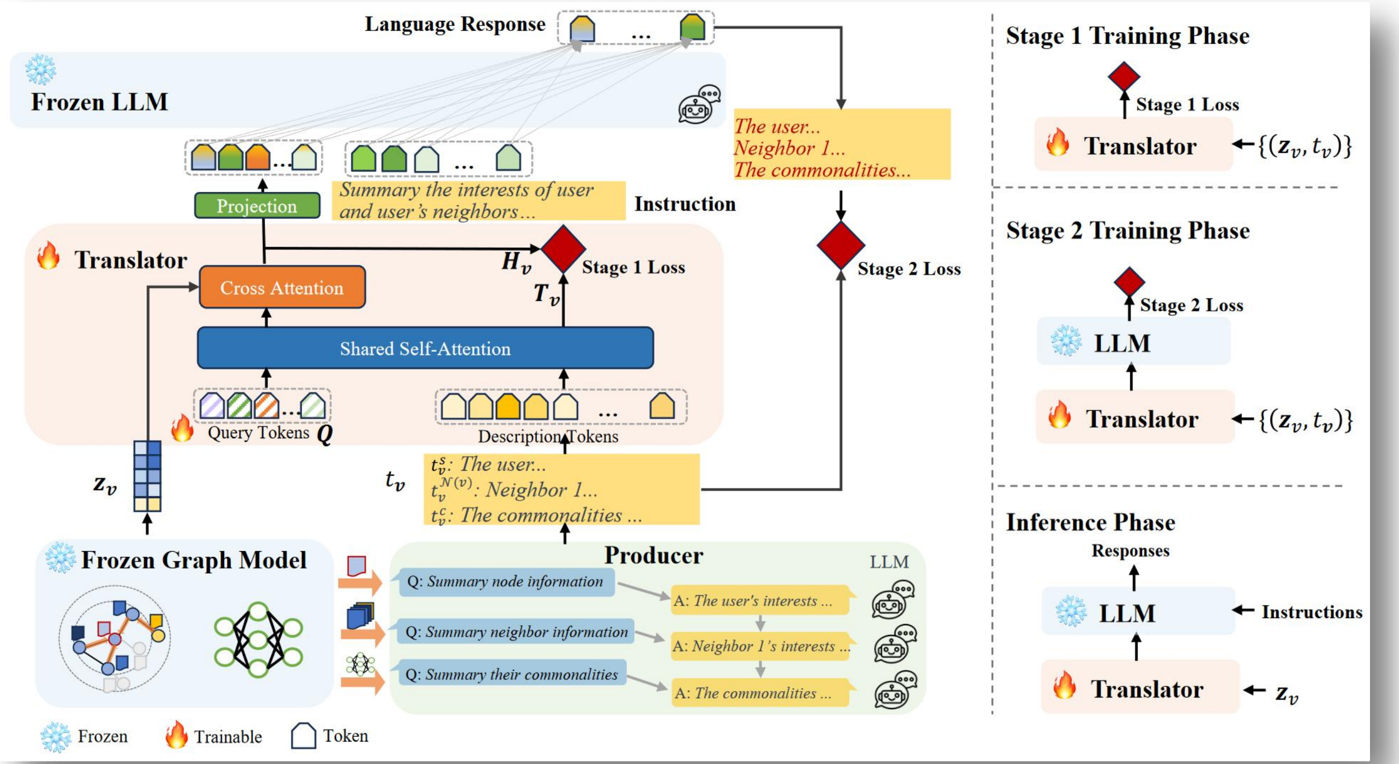
在三个维度上用LLM生成描述文本：

- 节点信息
- 邻居信息
- 模型信息

连接三个维度，得到节点描述文本t_v。

3. Translator

可学习查询标记Q与描述标记通过共享自注意力层交互信息，Q通过交叉注意力层与节点嵌入z_v进行交互。



$$H_v = f_z\{Q, z_v\}$$

$$T_v = BERT(t_v)$$

GraphTranslator: Aligning Graph Model to Large Language Model for Open-ended Tasks, WWW 2024

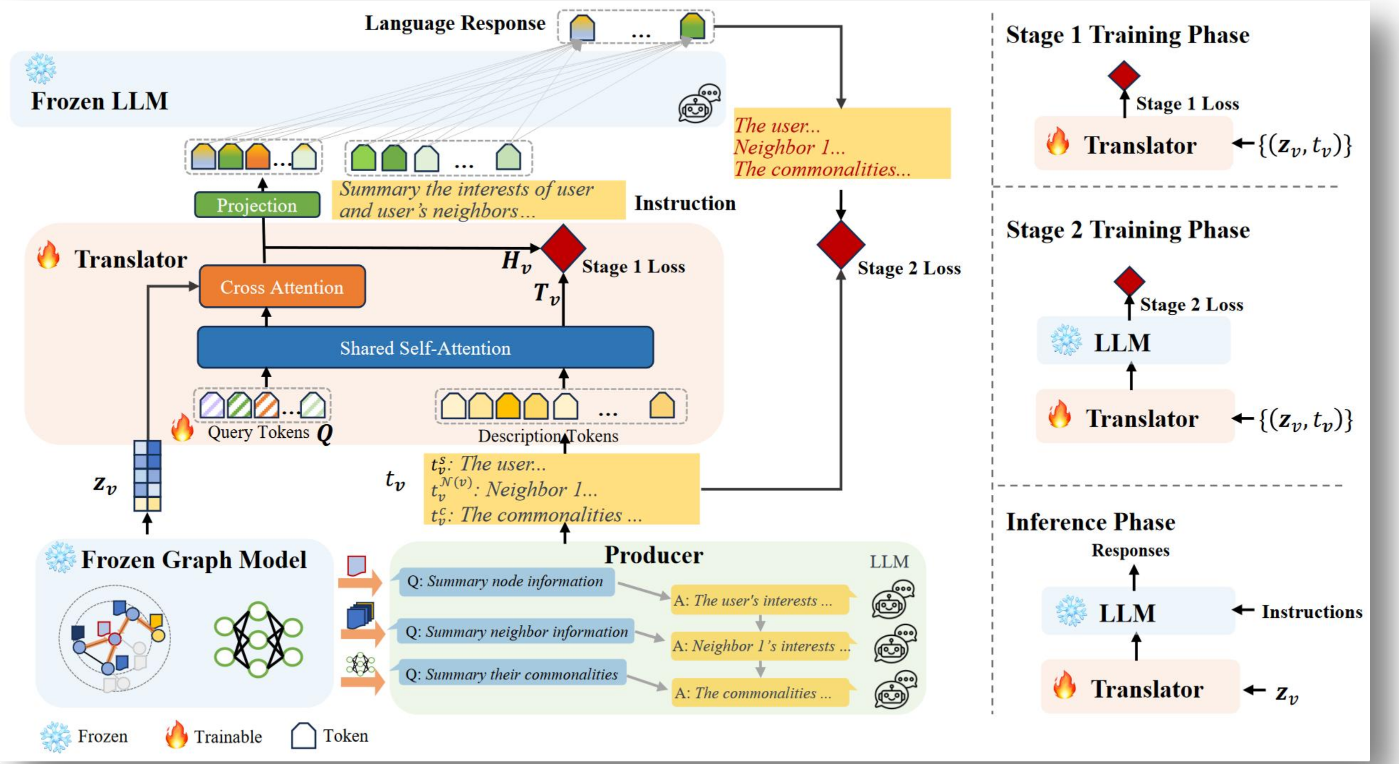
GNN→LLM Node-level

- **Training**

Stage 1：

通过优化三个目标来对齐文本表示T_v和节点嵌入H_v：

- 对比目标：计算文本表示和节点嵌入之间的成对相似度，选择最大的相似度作为相似度得分，然后将正负对的相似度进行对比。
- 生成目标：Q通过共享自注意力层与t_v通信，用交叉注意力层提取节点嵌入z_v中的信息，最小化文本表示T_v与生成文本之间的交叉熵损失，让Q被迫捕获节点嵌入中与文本描述更相关的部分。
- 匹配目标：将文本描述和节点表示连接，输入到二元分类器中来衡量之间的相似度。



Stage 2：

将H_v通过线性层投影到LLM的维度，通过人类指令和LLM生成新的文本描述，与旧文本描述进行对齐，更新参数。

GraphTranslator: Aligning Graph Model to Large Language Model for Open-ended Tasks, WWW 2024

GNN→LLM Node-level

- **Experiment (Pre-defined Tasks)**

Table 1: Results on zero-shot node classification.

Dataset	Metric	BERT	RoBERTa	BERT*	RoBERTa*	LLM+s_v	LLM+s_v+$s_{\mathcal{N}(v)}$	GraphTranslator
Taobao (Lifestage)	Legality Rate (%)	100.00	100.00	100.00	100.00	50.10	55.57	58.80
	Accuracy (%)	<u>34.73</u>	33.10	32.97	34.53	33.46	34.59	**35.33**
	Recall (%)	<u>34.73</u>	33.10	32.97	34.53	33.46	34.59	**35.33**
	Macro-F1 (%)	27.17	24.56	25.06	25.73	31.63	<u>32.60</u>	**32.62**
Taobao (Cat Owner)	Legality Rate (%)	100.00	100.00	100.00	100.00	31.20	45.43	98.97
	Accuracy (%)	51.13	50.87	49.03	48.77	<u>51.92</u>	**58.55**	50.99
	Recall (%)	<u>87.40</u>	60.40	63.27	11.73	12.82	45.56	**95.69**
	Macro-F1 (%)	43.73	50.42	47.98	40.62	21.05	<u>52.96</u>	**66.14**
Taobao (Vehicle Owner)	Legality Rate (%)	100.00	100.00	100.00	100.00	63.97	86.17	94.60
	Accuracy (%)	47.53	47.93	47.37	48.73	46.74	<u>49.09</u>	**49.40**
	Recall (%)	59.00	54.73	51.53	<u>64.60</u>	63.01	61.29	**83.27**
	Macro-F1 (%)	46.83	47.69	47.28	47.41	54.62	<u>55.15</u>	**61.87**
ArXiv	Legality Rate(%)	100.00	100.00	100.00	100.00	99.15	99.40	97.8
	Top-1 Acc (%)	1.63	3.55	14.53	6.95	14.07	<u>17.90</u>	**28.48**
	Top-3 Acc (%)	7.63	11.98	<u>29.60</u>	16.53	26.98	28.43	**37.62**
	Top-5 Acc (%)	28.00	22.93	38.30	23.75	**42.46**	37.99	<u>39.87</u>

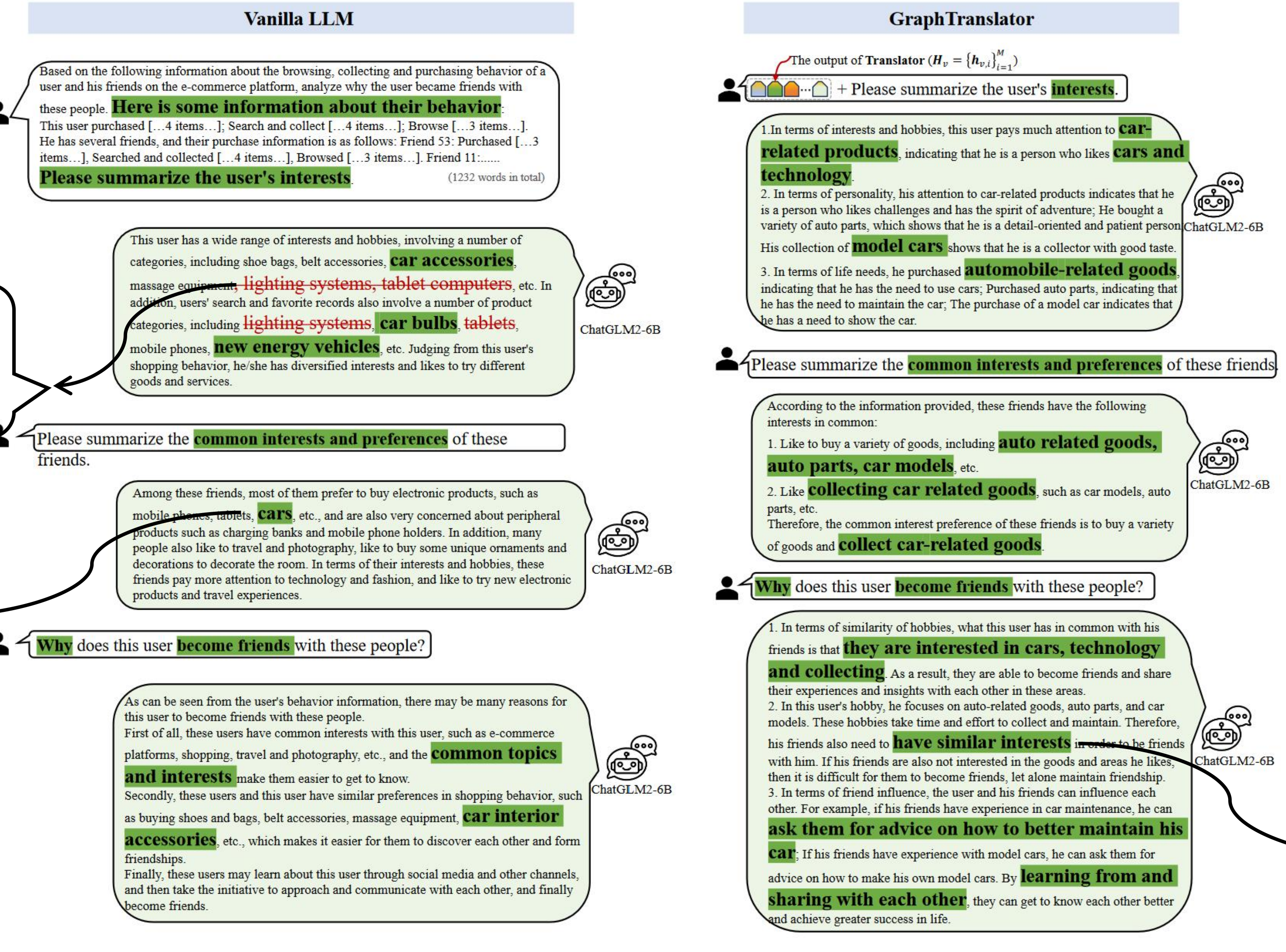
GraphTranslator: Aligning Graph Model to Large Language Model for Open-ended Tasks, WWW 2024

GNN→LLM Node-level

- **Experiment (Open-ended Tasks)**

属于friends的产品而不是user

太多冗余内容！



(a) Vanilla LLM: using text attribute of node and its neighbors as prompt

(b) GraphTranslator: using translated node embedding as prompt

从爱好相似度、友谊维系、朋友影响力三个角度进行解释

Figure 4: A case of graph question answering on Taobao Dataset.

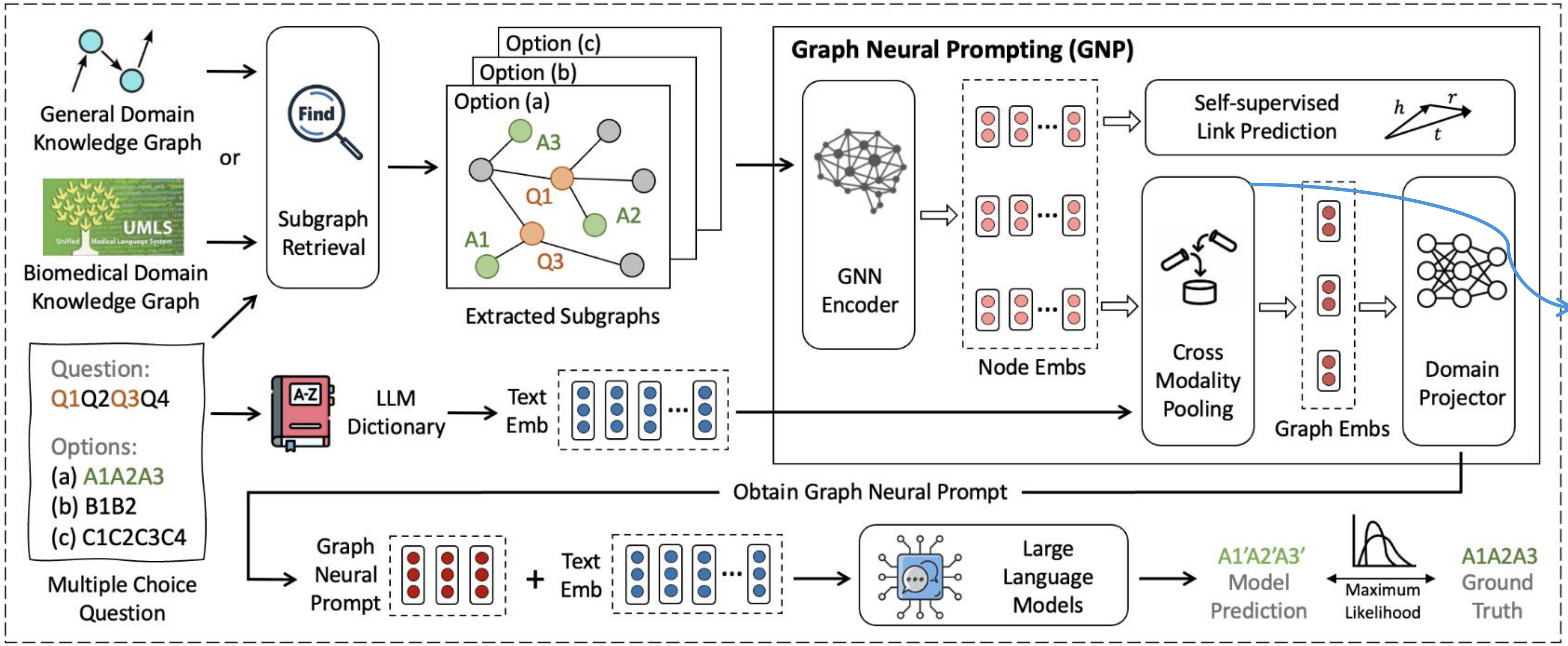
GraphTranslator: Aligning Graph Model to Large Language Model for Open-ended Tasks, WWW 2024

Graph Neural Prompting with Large Language Models

- **Motivation**

LLM 在准确捕获和返回基础知识方面具有局限性。现有的利用知识图谱进行检索增强的方法是将三元组直接输入LLM，但存在噪声。因此作者提出Graph Neural Prompting从知识图谱中学习**有用的知识**整合到LLM中。

- **Method**



Self-Attention
线性层维度匹配
跨模态注意力层
平均池化

Graph Neural Prompting with Large Language Models, AAAI 2024

GNN→LLM Graph-level

- **Experiment**

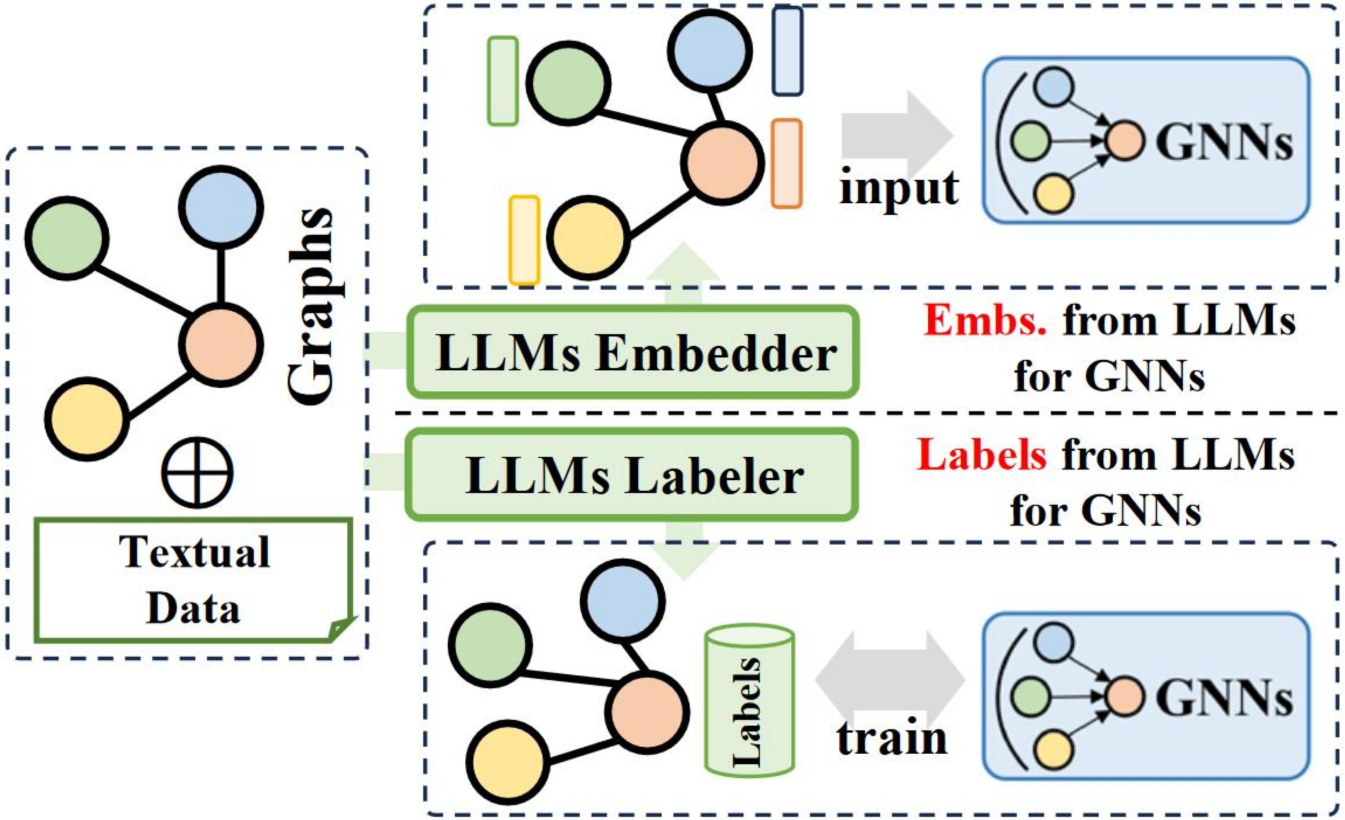
LLM	Setting	Method	Commonsense Reasoning				Biomedical Reasoning		Total
			OBQA	ARC	PIQA	Riddle	PQA	BioASQ	
FLAN-T5 xlarge (3B)	LLM Frozen	LLM-only	69.20	68.24	58.43	53.73	71.50	65.85	64.49
		Prompt Designs*	72.20	70.99	60.94	52.75	70.50	67.48	65.33
		KG Flattening REL	61.80	64.12	57.56	43.33	69.25	65.04	60.18
		KG Flattening BFS	62.80	63.86	56.69	44.12	69.25	65.04	60.29
		KAPING TH	58.80	63.52	52.34	40.78	70.00	65.04	58.41
		KAPING OH	60.00	63.09	51.69	41.37	70.00	65.04	58.53
		Prompt Tuning	72.20	70.64	60.83	53.33	72.00	66.67	65.95
		GNP	**79.80**	**71.85**	**61.48**	**66.86**	**76.75**	**89.43**	**74.36**
		Δ_{PT}	↑ 10.53%	↑ 1.71%	↑ 1.07%	↑ 25.37%	↑ 6.60%	↑ 34.14%	↑ 12.76%
	LLM Tuned	Full Fine-tuning	82.80	73.30	63.55	74.12	76.25	91.06	76.85
		LoRA	80.40	71.33	63.76	72.94	76.25	92.68	76.23
		LoRA + GNP	**83.40**	**72.45**	**64.31**	**75.49**	76.25	92.68	**77.43**
		Δ_{LoRA}	↑ 3.73%	↑ 1.57%	↑ 0.86%	↑ 3.50%	↑ 0.00%	↑ 0.00%	↑ 1.58%
FLAN-T5 xxlarge (11B)	LLM Frozen	LLM-only	76.80	68.93	56.58	61.37	71.75	65.85	66.88
		Prompt Designs*	79.60	74.16	58.00	60.59	71.25	66.67	68.38
		KG Flattening REL	72.80	66.78	56.80	53.53	69.50	66.67	64.35
		KG Flattening BFS	72.40	66.95	56.37	54.90	68.75	65.85	64.20
		KAPING TH	60.60	57.25	53.21	48.43	68.75	66.67	59.15
		KAPING OH	60.00	56.65	52.99	47.65	69.25	66.67	58.87
		Prompt Tuning	78.80	74.85	61.26	61.37	70.00	65.04	68.55
		GNP	**87.20**	**78.20**	**63.66**	**70.98**	**76.75**	**90.24**	**77.84**
		Δ_{PT}	↑ 10.66%	↑ 4.48%	↑ 3.92%	↑ 15.66%	↑ 9.64%	↑ 38.75%	↑ 13.54%
	LLM Tuned	Full Fine-tuning	89.40	76.82	65.61	80.78	78.00	92.68	80.55
		LoRA	88.60	78.54	65.61	74.90	77.75	91.06	79.41
		LoRA + GNP	**89.60**	**78.71**	**65.94**	**76.67**	**79.75**	**94.31**	**80.83**
		Δ_{LoRA}	↑ 1.13%	↑ 0.22%	↑ 0.50%	↑ 2.36%	↑ 2.57%	↑ 3.57%	↑ 1.79%

Graph Neural Prompting with Large Language Models, AAAI 2024

LLM→GNN

概述

- LLM强大的语言总结和建模能力为GNN提供初始嵌入。
- LLM生成监督信号来改进GNN的训练。 LLM的生成作为输入。 ×！



A Survey of Large Language Models for Graphs, KDD 2024

相关工作

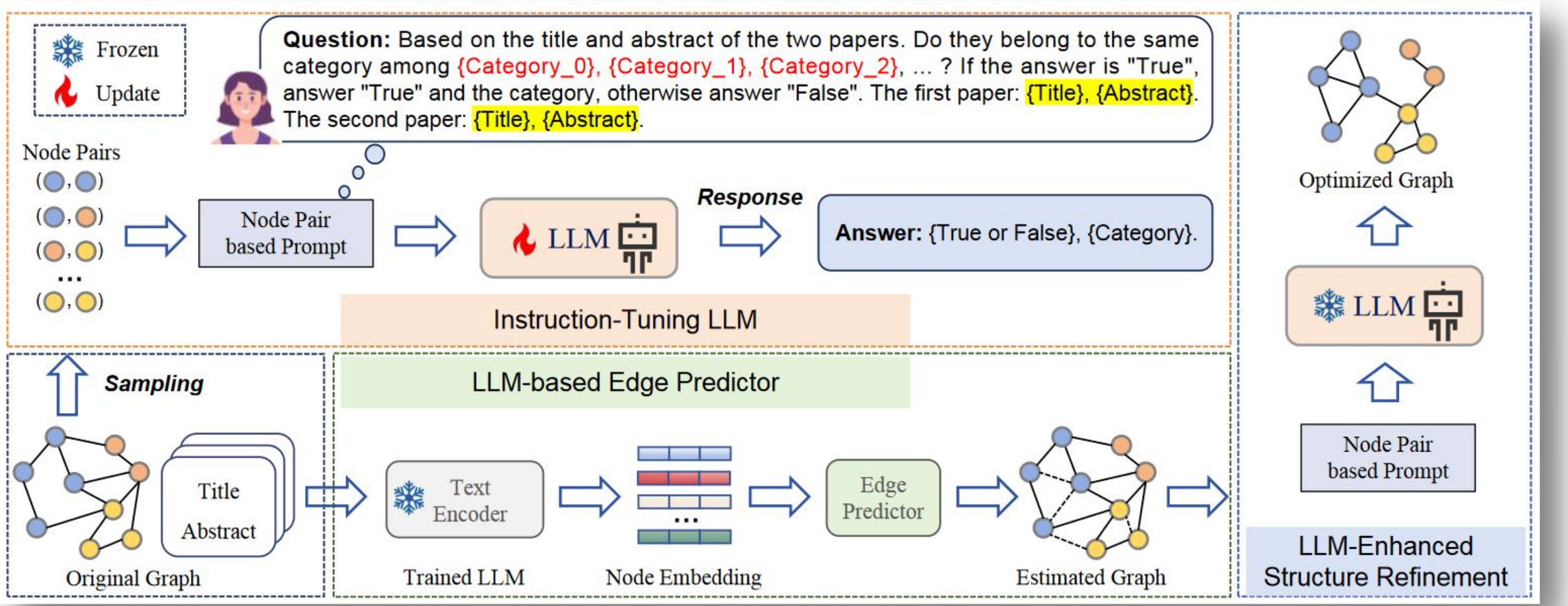
1. **LLMs-Labeler**
    - GraphEdit: Large Language Models for Graph Structure Learning
    - Label-free node classification on graphs with large language models (LLMs), ICLR 2024

GraphEdit: Large Language Models for Graph Structure Learning

- **Motivation**:

图结构学习GSL过度依赖作为监督信号的图结构信息，容易受到标签稀疏性和结构噪声的影响。
因此作者希望利用LLM去除噪声连接并识别节点间的潜在依赖关系。

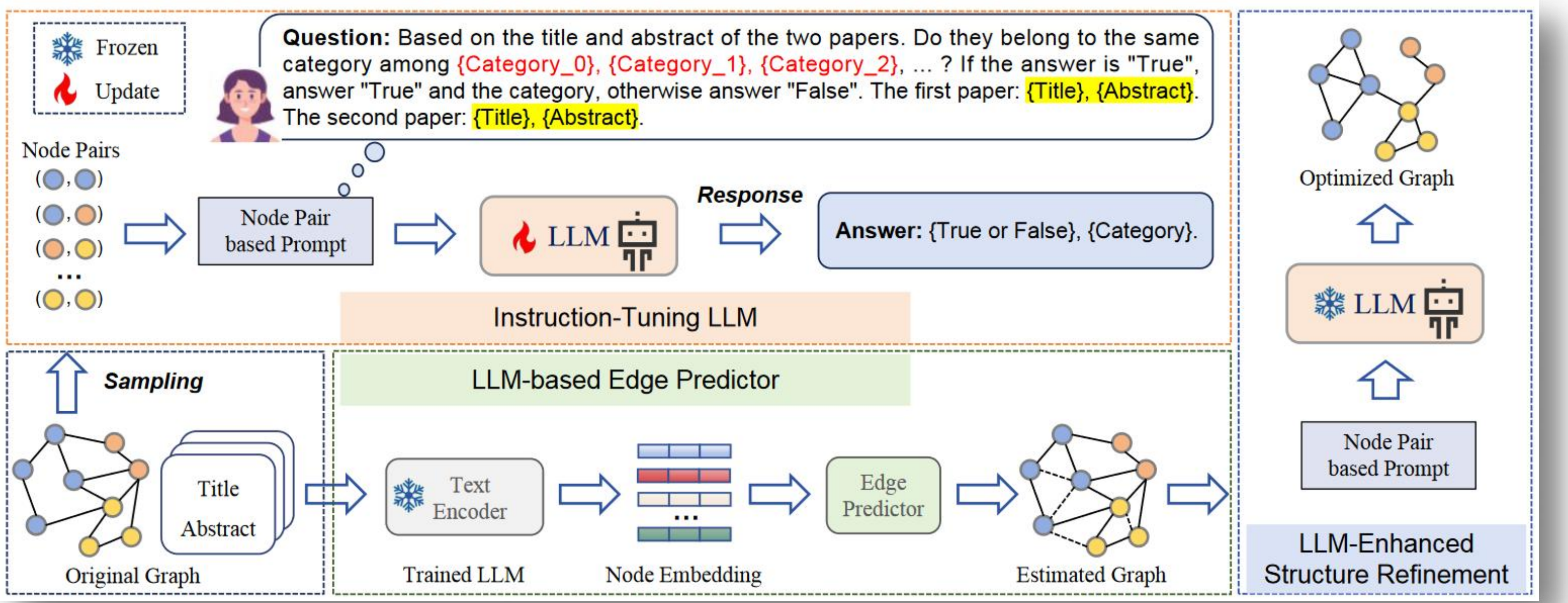
- **Method**:



GraphEdit: Large Language Models for Graph Structure Learning

LLM→GNN LLMs-Labeler

- **Method**:



Instruction-Tuning LLM:

利用LLM通过节点之间的语义识别潜在连接。

Prompt包含:

1. 节点对是否同类
2. 所属类别

LLM-based Edge Predictor:

节点对通过经过训练的LLM得到节点表示。连接节点表示，通过链接预测任务训练轻量级边预测器。

LLM-enhanced Structure Refinement:

边缘预测器选择前k个可能的候选边，候选边和原始边统一由LLM评估是否保留。

下游任务

GraphEdit: Large Language Models for Graph Structure Learning

LLM→GNN LLMs-Labeler

- **Experiment**

使用 Vicuna-v1.5 作为 LLM，并使用 LoRA 方法进行训练。

下游任务是节点分类。

Model	Cora	Citeseer	PubMed
GCN	87.36 ± 1.60	78.87 ± 2.18	87.37 ± 0.77
GRCN	84.13 ± 0.37	74.23 ± 1.18	85.20 ± 0.10
IDGL	88.63 ± 0.44	80.85 ± 0.07	88.30 ± 0.12
GAug	86.72 ± 0.63	77.61 ± 1.02	84.48 ± 0.37
GEN	86.53 ± 0.63	80.38 ± 0.72	87.04 ± 0.11
SLAPS	81.99 ± 1.57	73.17 ± 0.87	85.21 ± 0.18
GT	88.34 ± 0.35	78.46 ± 0.48	86.69 ± 0.19
CoGSL	82.07 ± 0.51	78.84 ± 0.11	OOM
WSGNN	89.59 ± 0.17	80.88 ± 0.48	87.17 ± 0.19
SUBLIME	85.04 ± 0.37	43.73 ± 7.08	86.03 ± 0.33
STABLE	88.75 ± 0.35	75.67 ± 0.98	86.30 ± 0.15
Nodeformer	88.56 ± 1.01	80.28 ± 0.57	87.93 ± 0.26
GSR	87.56 ± 1.19	78.77 ± 1.56	85.61 ± 0.55
SEGSL	87.49 ± 0.66	78.91 ± 0.52	87.57 ± 0.37
GraphEdit	**90.90 ± 1.16**	**81.85 ± 1.42**	**94.09 ± 0.28**

与其他大模型的对比：

Table 7: Performance comparison with other LLMs.

Model	Cora	Citeseer
GCN	87.36 ± 1.60	78.87 ± 2.18
ChatGPT 3.5	85.30 ± 2.15	78.76 ± 2.19
ERNIE-Bot-turbo	86.99 ± 1.50	79.20 ± 2.25
Vicuna-7B	87.47 ± 1.22	79.55 ± 2.17
BLOOMZ-7B	84.87 ± 1.58	79.47 ± 2.28
Llama-2-7B	84.83 ± 1.94	78.65 ± 1.93
ChatGLM2-6B	80.92 ± 2.53	74.47 ± 2.09
AquilaChat-7B	86.31 ± 2.05	78.17 ± 2.42
GraphEdit	**88.38 ± 1.06**	**80.03 ± 2.16**

GraphEdit: Large Language Models for Graph Structure Learning

Label-free node classification on graphs with large language models (LLMs)

- **Motivation**：

图模型结构复杂，人工标注昂贵且容易出错。

- **Method**：

选择易于标注的节点

↓

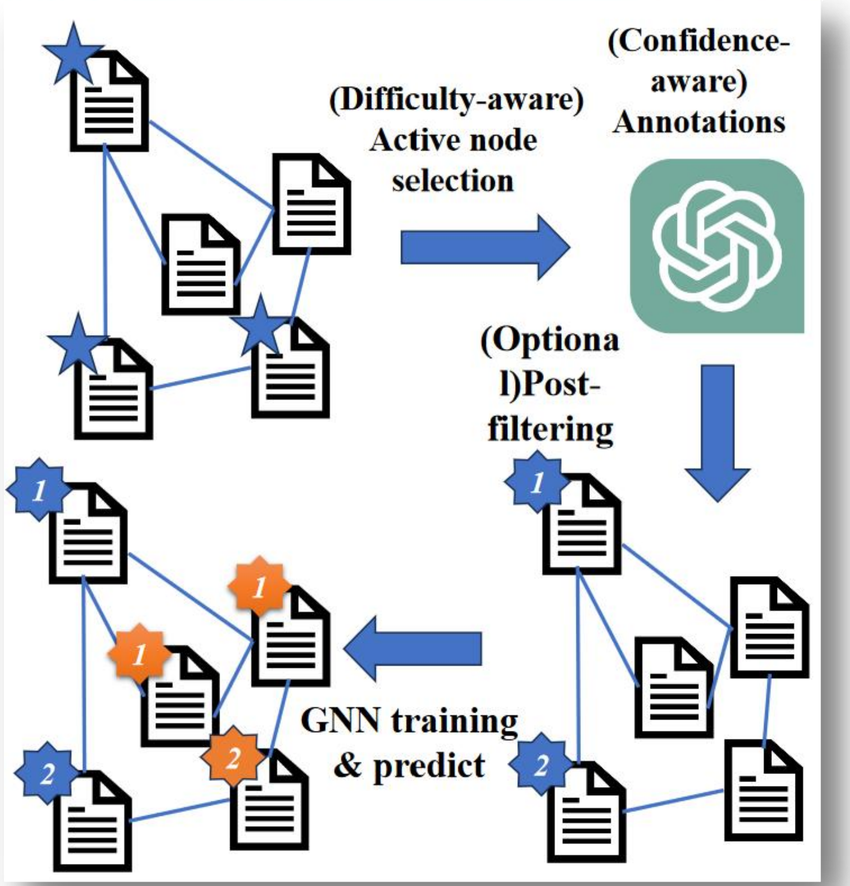
生成注释和置信度

↓

过滤低质量注释

↓

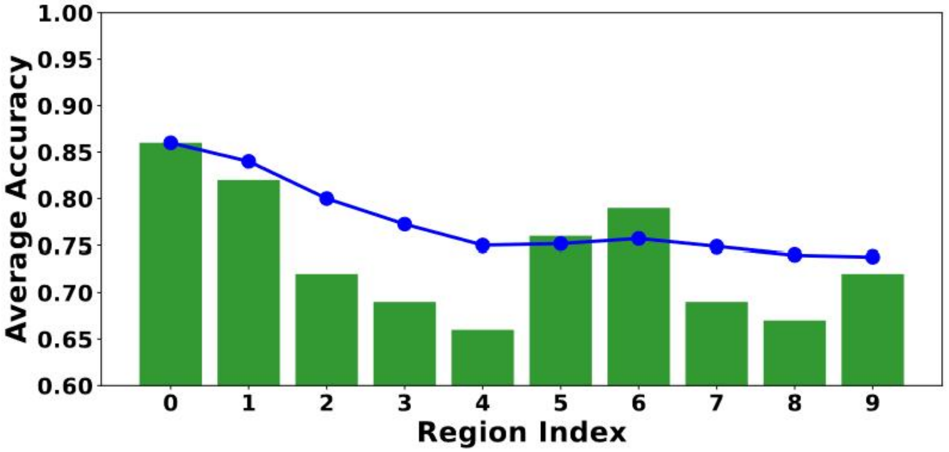
训练、预测



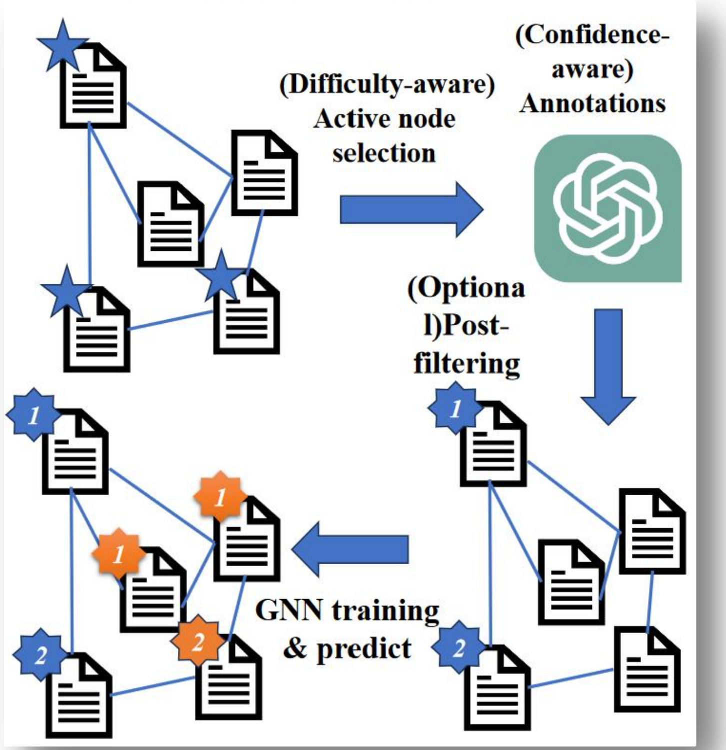
Label-free node classification on graphs with large language models (LLMs), ICLR 2024

- **Method**：

Difficulty-aware Active Node Selection：



(a) CORA



$$C - Density(v_i) = \frac{1}{1 + ||x_{v_i} - x_{CC_{v_i}}||}$$

$$f_{DA-act}(v_i) = \alpha_0 \times r_{f_{act}}(v_i) + \alpha_1 \times r_{C-Density}(v_i)$$

传统节点选择　　基于聚类节点密度

Label-free node classification on graphs with large language models (LLMs), ICLR 2024

LLM→GNN LLMs-Labeler

- **Experiment**

不同主动选择策略的准确性：

	Cora	Citeseer	Pubmed	WikiCS	ogbn-arxiv	ogbn-products
Random	70.48± 0.73	65.11 ± 1.12	72.98 ± 2.15	60.69 ± 1.73	64.59 ± 0.16	70.40 ± 0.60
Random-W	71.77± 0.75	65.92 ± 1.05	73.92 ± 1.75	61.42± 1.54	64.95 ± 0.19	71.96± 0.59
C-Density	42.22 ± 1.59	66.44 ± 0.34	74.43 ± 0.28	57.77 ± 0.85	44.08 ± 0.39	8.29 ± 0.00
PS-Random-W	72.38 ± 0.72	67.18 ± 0.92	73.31 ± 1.65	62.60 ± 0.94	65.22 ± 0.15	71.62± 0.54
Density	72.40 ± 0.35	61.06 ± 0.95	74.43 ± 0.28	64.96 ± 0.53	51.77 ± 0.24	20.22 ± 0.11
Density-W	72.39± 0.34	59.88 ± 0.97	73.00 ± 0.19	63.80 ± 0.69	51.03 ± 0.27	20.97 ± 0.15
DA-Density	70.73 ± 0.32	62.92 ±1.05	74.43 ± 0.28	63.08 ± 0.45	51.33 ± 0.29	8.50 ± 0.32
PS-Density-W	74.61 ± 0.13	61.00 ± 0.55	74.50 ± 0.23	65.57 ± 0.45	51.73 ± 0.29	19.15 ± 0.18
DA-Density-W	67.29 ± 0.96	62.98 ± 0.77	73.39 ± 0.35	63.26 ± 0.62	51.36 ± 0.39	8.52 ± 0.11
AGE	69.15 ± 0.38	54.25 ± 0.31	74.55 ± 0.54	55.51 ± 0.12	46.68 ± 0.30	65.63 ± 0.15
AGE-W	69.70 ± 0.45	57.60 ± 0.35	64.30 ± 0.49	55.15 ± 0.14	47.84± 0.35	64.92 ± 0.19
DA-AGE	74.38 ± 0.24	59.92 ± 0.42	74.20 ± 0.51	59.39 ± 0.21	48.21 ± 0.35	60.03 ± 0.11
PS-AGE-W	72.61 ± 0.39	57.44 ± 0.49	64.00 ± 0.44	56.13 ± 0.11	47.12 ± 0.39	68.62 ± 0.15
DA-AGE-W	74.96 ± 0.22	58.41 ± 0.45	65.85 ± 0.67	59.19 ± 0.24	47.79± 0.32	59.95 ± 0.23
RIM	69.86 ± 0.38	63.44 ± 0.42	76.22 ± 0.16	66.72± 0.16	OOT	OOT
DA-RIM	73.99 ± 0.44	60.33 ± 0.40	79.17 ± 0.11	67.82± 0.32	OOT	OOT
PS-RIM-W	73.19 ± 0.45	62.85 ± 0.49	74.52 ± 0.19	69.84 ± 0.19	OOT	OOT
DA-RIM-W	74.73 ± 0.41	60.80 ± 0.57	77.94 ± 0.24	68.22 ± 0.25	OOT	OOT
GraphPart	68.57 ± 2.18	66.59 ± 1.34	77.50 ± 1.23	67.28 ± 0.87	OOT	OOT
GraphPart-W	69.90 ± 2.03	68.20 ± 1.42	78.91 ± 1.04	68.43 ± 0.92	OOT	OOT
DA-GraphPart	69.35 ± 1.92	69.37 ± 1.27	79.49 ± 0.85	68.72 ± 1.01	OOT	OOT
PS-GraphPart-W	69.92± 1.75	69.06 ± 1.19	78.84 ± 1.05	66.90 ± 1.05	OOT	OOT
DA-GraphPart-W	68.61 ± 1.32	68.82 ± 1.17	79.89 ± 0.79	67.13 ± 1.23	OOT	OOT
FeatProp	72.82 ± 0.08	66.61 ± 0.55	73.90 ± 0.15	64.08 ± 0.12	66.06 ± 0.07	74.04 ± 0.15
FeatProp-W	73.56 ± 0.13	68.04 ± 0.69	76.90 ± 0.19	63.80 ± 0.21	66.32 ± 0.15	74.32 ± 0.14
PS-FeatProp	75.54 ± 0.34	69.06 ± 0.32	74.98 ± 0.35	66.09 ± 0.35	66.14 ± 0.27	74.91 ± 0.17
PS-FeatProp-W	76.23 ± 0.07	68.64 ± 0.71	78.84 ± 1.05	64.72 ± 0.19	65.84 ± 0.19	74.54 ± 0.24

Label-free node classification on graphs with large language models (LLMs), ICLR 2024

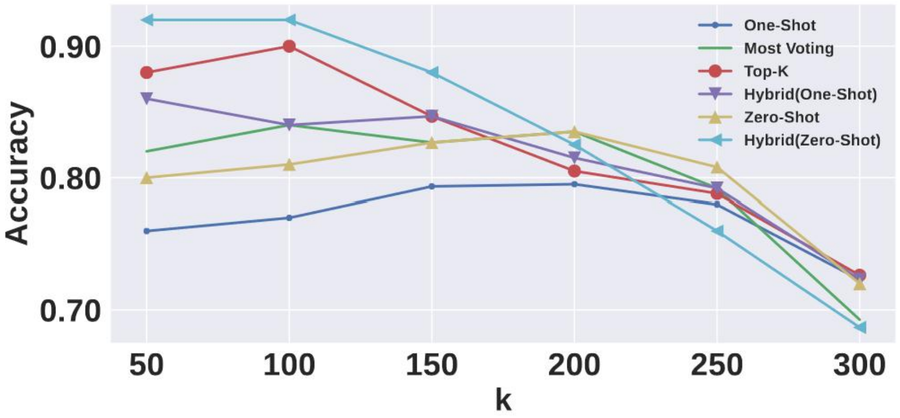
LLM→GNN LLMs-Labeler

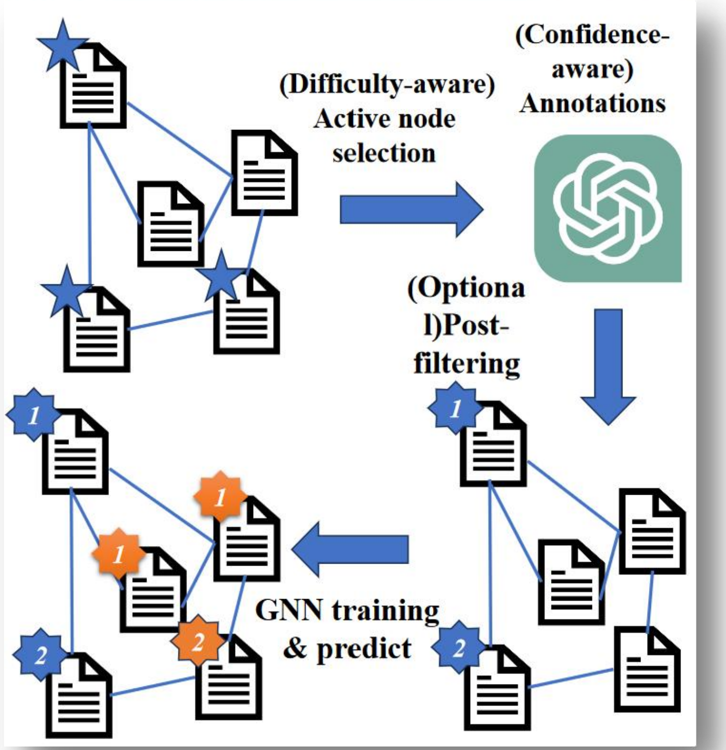
- **Method**：

Confidence-aware Annotations：

选择策略让LLM进行生成标注&置信度。

Prompt Strategy	CORA Acc (%)	CORA Cost	OGBN-PRODUCTS Acc (%)	OGBN-PRODUCTS Cost	WIKICS Acc (%)	WIKICS Cost
Vanilla (zero-shot)	68.33 ± 6.55	1	75.33 ± 4.99	1	68.33 ± 1.89	1
Vanilla (one-shot)	69.67 ± 7.72	2.2	78.67 ± 4.50	1.8	72.00 ± 3.56	2.4
TopK (zero-shot)	68.00 ± 6.38	1.1	74.00 ± 5.10	1.2	72.00 ± 2.16	1.1
Most Voting (zero-shot)	68.00 ± 7.35	1.1	75.33 ± 4.99	1.1	69.00 ± 2.16	1.1
Hybrid (zero-shot)	67.33 ± 6.80	1.5	73.67 ± 5.25	1.4	71.00 ± 2.83	1.4
Hybrid (one-shot)	70.33 ± 6.24	2.9	75.67 ± 6.13	2.3	73.67 ± 2.62	2.9





Hybrid(zero-shot) ✓

Label-free node classification on graphs with large language models (LLMs), ICLR 2024

LLM→GNN LLMs-Labeler

- **Method**:

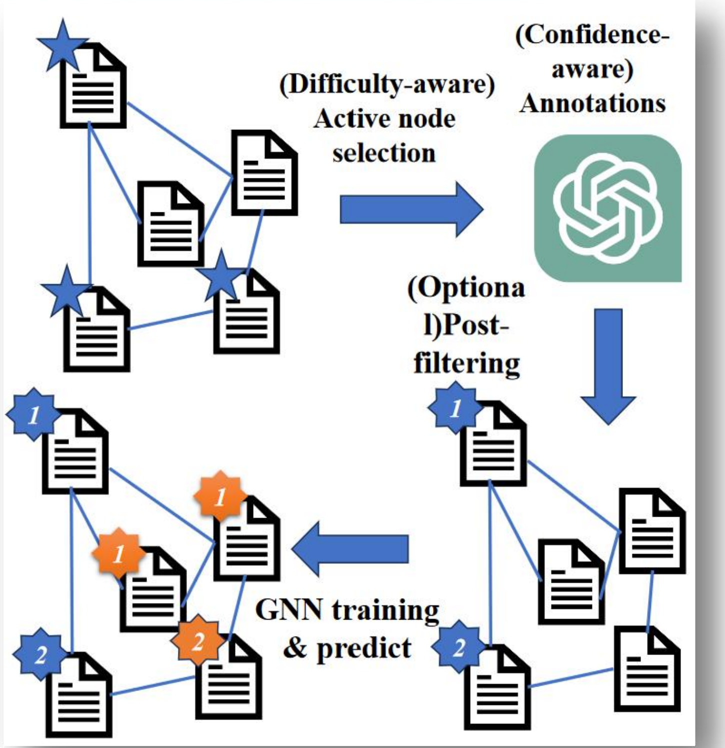
Post-filtering:

熵评分函数变化:

$$\mathrm{COE}(v_i) = \mathrm{H}(\tilde{y}_{V_{sel}-\{v_i\}}) - \mathrm{H}(\tilde{y}_{V_{sel}}) \qquad \uparrow$$

过滤得分函数:

$$f_{filter}(v_i) = \underbrace{\beta_0 \times r_{f_{conf}}(v_i)}_{\text{置信度}} + \underbrace{\beta_1 \times r_{COE}(v_i)}_{\text{熵评分}} + \underbrace{\beta_2 \times r_{C-Density}(v_i)}_{\text{聚类密度}}$$



Training & Prediction:

采用加权交叉熵损失，用置信度分数作为相应的权重。

Label-free node classification on graphs with large language models (LLMs), ICLR 2024

LLM→GNN LLMs-Labeler

- **Experiment**

与其他无标签节点分类的比较：

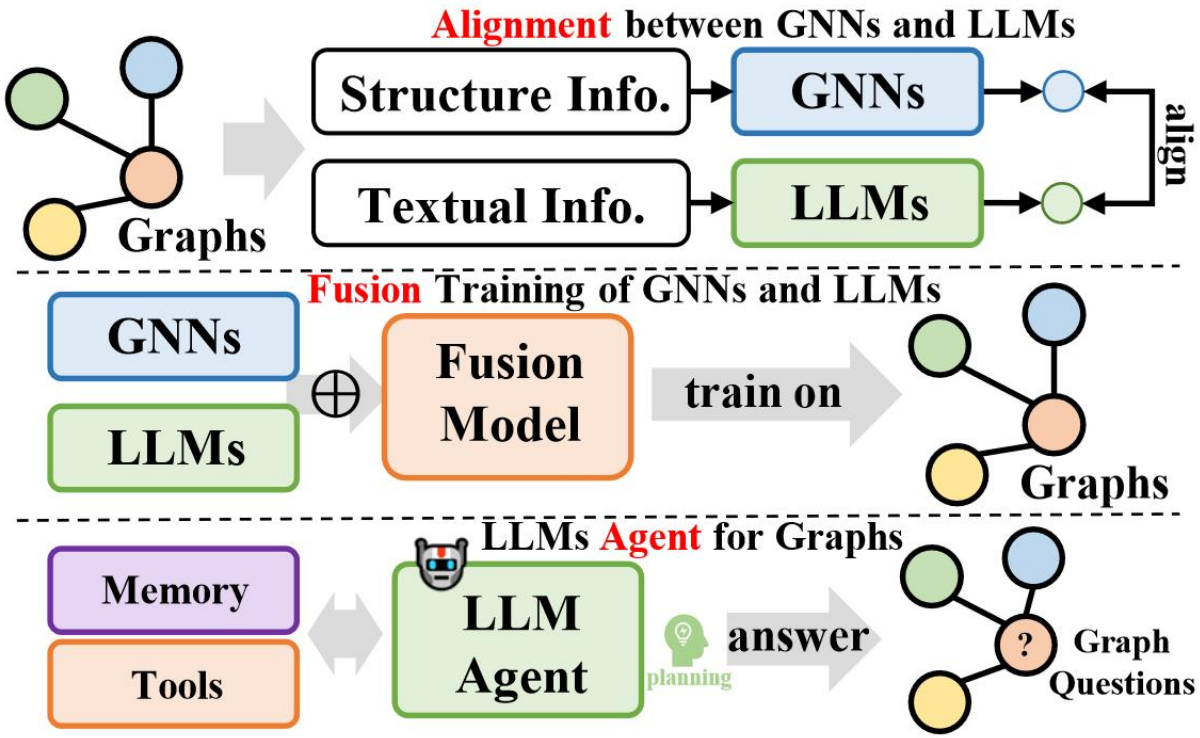
	OGBN-ARXIV		OGBN-PRODUCTS	
Methods	Acc	Cost	Acc	Cost
SES(*)	13.08	N/A	6.67	N/A
TAG-Z(*)	37.08	N/A	47.08	N/A
BART-large-MNLI	13.2	N/A	28.8	N/A
LLMs-as-Predictors	73.33	79	75.33	1572
LLM-GNN	66.32	0.63	74.91	0.74

Label-free node classification on graphs with large language models (LLMs), ICLR 2024

LLMs-Graphs Intergration

概述

- 对齐LLM和GNN的特征空间，增强LLM处理图数据的能力，同时增强GNN参数学习的能力。
- 通过设计模块实现更高级别的融合。



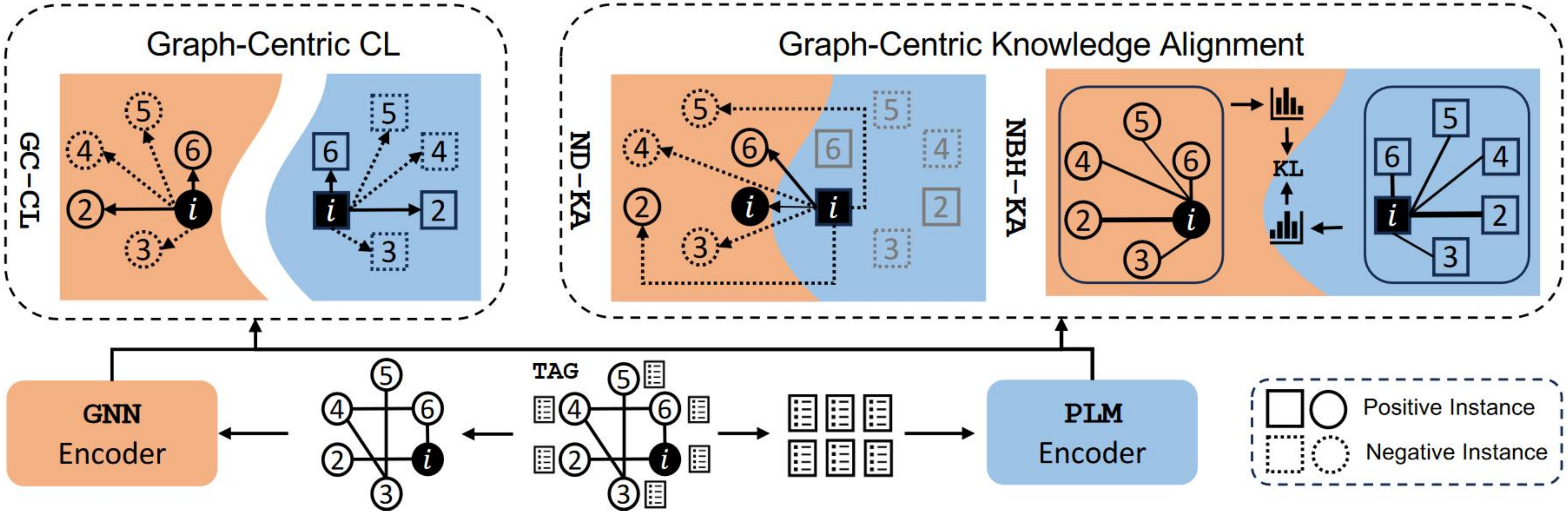
A Survey of Large Language Models for Graphs, KDD 2024

相关工作

1. **Alignment between GNNs and LLMs**
   - Grenade: Graph-Centric Language Model for Self-Supervised Representation Learning on Text-Attributed Graphs

Grenade: Graph-Centric Language Model for Self-Supervised Representation Learning on Text-Attributed Graphs

- **Method**

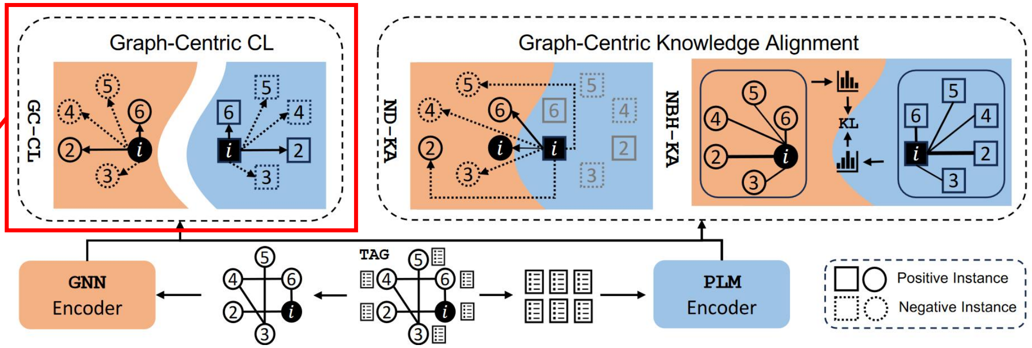


Grenade: Graph-Centric Language Model for Self-Supervised Representation Learning on Text-Attributed Graphs

- **Method**

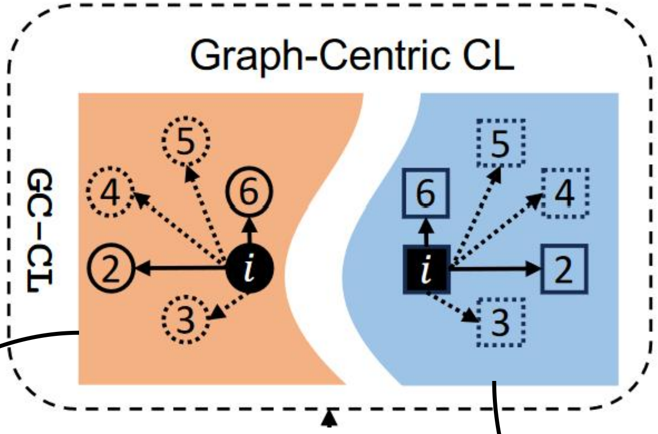
Graph-Centric Contrastive Learning：

相邻节点共享相似的语义



正例N(i)：节点i的k跳邻节点

负例B(i)：除节点i的小批量实例



$$C(i) = N(i) \cup B(i)$$

对于图模型：

$$L_{GC-CL_2} = -\frac{1}{|N(i)|}\sum_{p\in N(i)} log \frac{e^{sim(e_i, e_p)/\tau}}{\sum_{j\in C(i)} e^{sim(e_i, e_j)/\tau}}$$

对于语言模型：

$$L_{GC-CL_1} = -\frac{1}{|N(i)|}\sum_{p\in N(i)} log \frac{e^{sim(d_i, d_p)/\tau}}{\sum_{j\in C(i)} e^{sim(d_i, d_j)/\tau}}$$

Grenade: Graph-Centric Language Model for Self-Supervised Representation Learning on Text-Attributed Graphs

- **Method**

Dual-level Graph-Centric Knowledge Alignment：

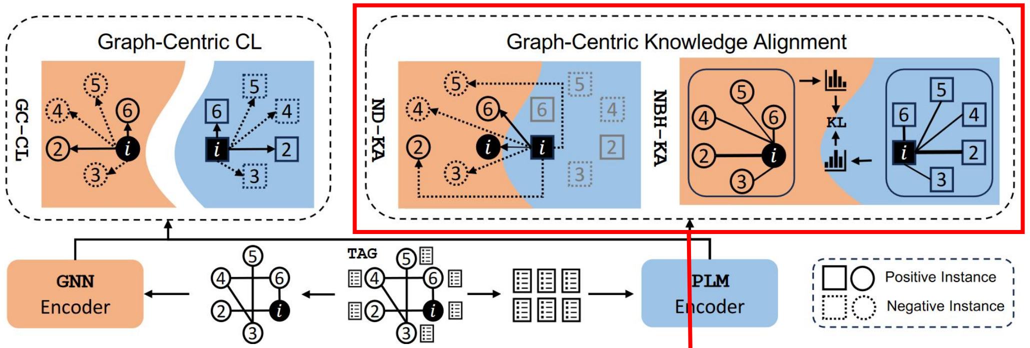
节点级知识对齐：

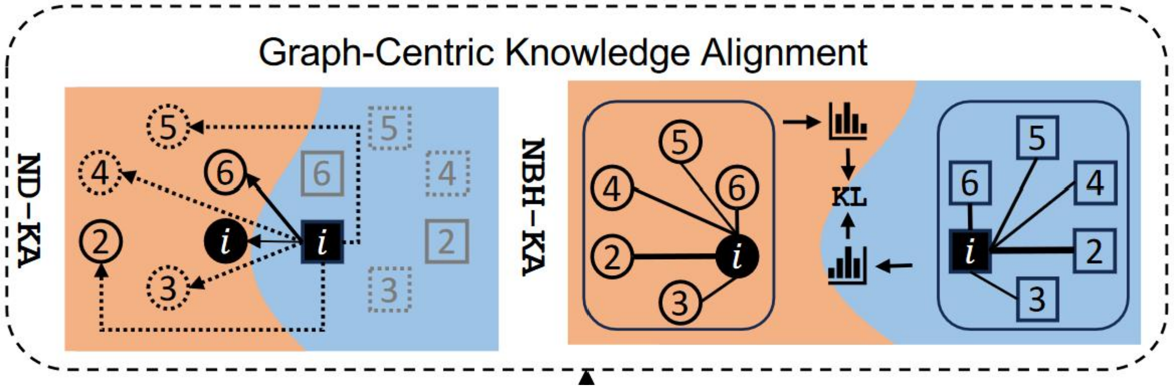
正例$\widetilde{N}(\mathrm{i})$：节点i的k跳邻节点+节点i

负例B(i)：除节点i的小批量实例

$$\widetilde{C}(\mathrm{i}) = \widetilde{N}(\mathrm{i}) \cup \mathrm{B}(\mathrm{i})$$

$$L_{ND-KA} = - \frac{1}{|\widetilde{N}(i)|} \sum_{p \in \widetilde{N}(i)} \left(\log \frac{e^{sim(e_i, d_p)/\tau}}{\sum_{j \in \widetilde{C}(i)} e^{sim(e_i, d_j)/\tau}} + \log \frac{e^{sim(d_i, e_p)/\tau}}{\sum_{j \in \widetilde{C}(i)} e^{sim(d_i, e_j)/\tau}} \right)/2$$





邻域级知识对齐：

$$P_{PLM}(i) = softmax_{j \in C(i)}(sim(d_i, d_j)/\tau)$$

$$P_{GNN}(i) = softmax_{j \in C(i)}(sim(e_i, e_j)/\tau)$$

$$L_{NBH-KA} = (KL(P_{PLM}(i)||P_{GNN}(i)) + KL(P_{GNN}(i)||P_{PLM}(i)))/2$$

$$L = L_{GC-CL_1} + L_{GC-CL_2} + L_{ND-KA} + L_{NBH-KA}$$

Grenade: Graph-Centric Language Model for Self-Supervised Representation Learning on Text-Attributed Graphs

LLMs-Graphs Intergration   Alignment between GNNs and LLMs

- **Experiment**

Few-shot Node Classification

Methods	MLP $k=2$	MLP $k=4$	MLP $k=8$	MLP $k=16$	GraphSAGE $k=2$	GraphSAGE $k=4$	GraphSAGE $k=8$	GraphSAGE $k=16$
ogbn-arxiv								
OGB*	32.16$_{\pm 1.96}$	37.81$_{\pm 1.62}$	42.33$_{\pm 1.07}$	45.84$_{\pm 0.47}$	49.91$_{\pm 3.46}$	55.52$_{\pm 1.42}$	59.30$_{\pm 1.14}$	62.21$_{\pm 0.58}$
BERT	34.06$_{\pm 2.73}$	40.29$_{\pm 2.16}$	46.59$_{\pm 0.88}$	50.17$_{\pm 1.02}$	52.92$_{\pm 3.21}$	57.11$_{\pm 1.06}$	60.36$_{\pm 1.17}$	64.10$_{\pm 0.61}$
BERT+MLM	38.41$_{\pm 2.11}$	46.72$_{\pm 1.72}$	51.89$_{\pm 0.98}$	55.87$_{\pm 1.23}$	53.02$_{\pm 1.26}$	57.76$_{\pm 1.41}$	61.94$_{\pm 0.77}$	65.22$_{\pm 0.49}$
SimCSE	28.83$_{\pm 1.68}$	32.65$_{\pm 1.46}$	37.78$_{\pm 1.26}$	43.25$_{\pm 0.69}$	46.61$_{\pm 2.97}$	53.86$_{\pm 1.20}$	57.75$_{\pm 0.89}$	62.39$_{\pm 0.61}$
SPECTER	50.15$_{\pm 2.21}$	54.46$_{\pm 0.96}$	58.74$_{\pm 0.63}$	61.63$_{\pm 0.78}$	53.85$_{\pm 2.27}$	59.46$_{\pm 1.63}$	63.43$_{\pm 0.61}$	66.41$_{\pm 0.45}$
GIANT*	48.50$_{\pm 2.30}$	55.72$_{\pm 1.90}$	59.80$_{\pm 1.03}$	64.15$_{\pm 0.87}$	50.18$_{\pm 2.46}$	55.30$_{\pm 1.69}$	59.24$_{\pm 1.33}$	63.48$_{\pm 0.77}$
GLEM	-	-	-	-	27.14$_{\pm 2.31}$	45.52$_{\pm 1.27}$	53.37$_{\pm 1.08}$	55.39$_{\pm 0.89}$
GRENADE	**55.85**$_{\pm 2.34}$	**61.10**$_{\pm 1.59}$	**63.95**$_{\pm 0.89}$	**66.62**$_{\pm 0.47}$	**57.17**$_{\pm 3.54}$	**60.49**$_{\pm 0.93}$	**64.65**$_{\pm 1.08}$	**67.50**$_{\pm 0.41}$
ogbn-products								
OGB*	9.47$_{\pm 1.51}$	13.54$_{\pm 1.42}$	16.83$_{\pm 2.63}$	20.71$_{\pm 1.32}$	24.74$_{\pm 3.01}$	33.14$_{\pm 2.58}$	38.38$_{\pm 1.18}$	44.19$_{\pm 2.61}$
BERT	20.53$_{\pm 4.03}$	30.91$_{\pm 2.64}$	40.82$_{\pm 1.52}$	47.77$_{\pm 1.07}$	40.53$_{\pm 2.87}$	50.43$_{\pm 1.73}$	57.29$_{\pm 1.48}$	59.03$_{\pm 0.48}$
BERT+MLM	38.54$_{\pm 3.35}$	47.15$_{\pm 3.41}$	55.95$_{\pm 0.89}$	59.57$_{\pm 1.53}$	54.73$_{\pm 4.35}$	60.80$_{\pm 2.65}$	64.63$_{\pm 1.94}$	67.75$_{\pm 1.48}$
SimCSE	7.76$_{\pm 1.22}$	11.30$_{\pm 1.30}$	17.94$_{\pm 1.91}$	25.61$_{\pm 0.72}$	24.99$_{\pm 5.01}$	37.05$_{\pm 1.73}$	44.74$_{\pm 1.96}$	50.13$_{\pm 2.94}$
SPECTER	27.86$_{\pm 4.14}$	43.70$_{\pm 2.70}$	51.51$_{\pm 1.54}$	57.63$_{\pm 1.45}$	42.74$_{\pm 4.58}$	51.91$_{\pm 2.31}$	57.72$_{\pm 2.52}$	60.77$_{\pm 1.36}$
GIANT*	20.83$_{\pm 2.68}$	31.37$_{\pm 1.95}$	42.84$_{\pm 2.72}$	51.36$_{\pm 2.19}$	30.90$_{\pm 4.63}$	40.80$_{\pm 4.01}$	52.34$_{\pm 2.20}$	58.58$_{\pm 2.36}$
GLEM	-	-	-	-	41.72$_{\pm 4.62}$	42.50$_{\pm 3.45}$	43.05$_{\pm 2.78}$	48.64$_{\pm 2.01}$
GRENADE	**38.60**$_{\pm 4.51}$	**49.64**$_{\pm 1.39}$	**59.34**$_{\pm 2.38}$	**65.05**$_{\pm 1.00}$	**59.63**$_{\pm 2.80}$	**64.95**$_{\pm 1.63}$	**67.38**$_{\pm 2.17}$	**70.92**$_{\pm 1.18}$
ogbl-citation2								
OGB*	21.78$_{\pm 1.55}$	25.54$_{\pm 1.55}$	27.39$_{\pm 0.69}$	29.53$_{\pm 0.70}$	18.83$_{\pm 3.12}$	22.49$_{\pm 1.84}$	31.38$_{\pm 1.89}$	35.19$_{\pm 0.89}$
BERT	17.95$_{\pm 2.34}$	20.84$_{\pm 2.17}$	23.84$_{\pm 1.36}$	26.77$_{\pm 1.38}$	21.05$_{\pm 2.49}$	25.65$_{\pm 1.58}$	28.06$_{\pm 2.03}$	35.84$_{\pm 1.48}$
BERT+MLM	32.03$_{\pm 1.84}$	34.39$_{\pm 2.61}$	38.53$_{\pm 1.82}$	41.66$_{\pm 0.98}$	26.28$_{\pm 2.35}$	28.10$_{\pm 2.47}$	37.69$_{\pm 1.39}$	42.63$_{\pm 1.21}$
SimCSE	13.27$_{\pm 1.08}$	16.68$_{\pm 0.62}$	20.01$_{\pm 1.03}$	23.57$_{\pm 0.77}$	20.01$_{\pm 2.04}$	28.11$_{\pm 2.90}$	28.17$_{\pm 1.06}$	31.71$_{\pm 1.28}$
SPECTER	30.81$_{\pm 2.94}$	35.31$_{\pm 1.92}$	39.74$_{\pm 1.33}$	42.31$_{\pm 0.64}$	31.57$_{\pm 2.04}$	35.66$_{\pm 2.18}$	37.23$_{\pm 2.70}$	45.59$_{\pm 1.82}$
GIANT*	38.93$_{\pm 1.81}$	43.74$_{\pm 1.93}$	48.81$_{\pm 1.25}$	52.05$_{\pm 0.72}$	35.75$_{\pm 2.72}$	38.43$_{\pm 3.43}$	40.99$_{\pm 3.42}$	49.44$_{\pm 1.68}$
GLEM	-	-	-	-	30.86$_{\pm 4.62}$	33.78$_{\pm 1.88}$	47.36$_{\pm 2.73}$	51.42$_{\pm 1.41}$
GRENADE	**46.40**$_{\pm 2.00}$	**47.93**$_{\pm 1.34}$	**50.61**$_{\pm 0.71}$	**53.75**$_{\pm 0.82}$	**40.63**$_{\pm 3.77}$	**44.44**$_{\pm 2.63}$	**49.15**$_{\pm 1.73}$	**52.41**$_{\pm 1.94}$

Grenade: Graph-Centric Language Model for Self-Supervised Representation Learning on Text-Attributed Graphs

- **Experiment**

Node Clustering

Methods	ogbn-arxiv ACC	ogbn-arxiv ARI	ogbn-arxiv NMI	ogbn-products ACC	ogbn-products ARI	ogbn-products NMI	ogbl-citation2 ACC	ogbl-citation2 ARI	ogbl-citation2 NMI
OGB	$39.57_{\pm 0.39}$	$12.76_{\pm 1.22}$	$17.43_{\pm 0.79}$	$38.53_{\pm 1.43}$	$16.46_{\pm 4.24}$	$20.21_{\pm 1.84}$	$40.31_{\pm 0.40}$	$22.82_{\pm 0.34}$	$40.57_{\pm 0.38}$
BERT	$35.65_{\pm 1.21}$	$8.41_{\pm 1.01}$	$12.78_{\pm 1.20}$	$48.72_{\pm 0.57}$	$52.17_{\pm 1.81}$	$35.76_{\pm 0.82}$	$40.57_{\pm 0.31}$	$22.58_{\pm 0.84}$	$33.38_{\pm 0.44}$
BERT+MLM	$40.07_{\pm 0.60}$	$15.05_{\pm 0.17}$	$19.24_{\pm 0.51}$	$64.35_{\pm 0.81}$	$69.58_{\pm 1.31}$	$54.64_{\pm 0.31}$	$49.13_{\pm 0.46}$	$31.91_{\pm 0.46}$	$44.44_{\pm 0.34}$
SimCSE	$33.42_{\pm 0.74}$	$5.80_{\pm 0.40}$	$9.62_{\pm 0.74}$	$39.40_{\pm 1.02}$	$29.00_{\pm 2.22}$	$19.88_{\pm 1.01}$	$26.67_{\pm 0.64}$	$8.49_{\pm 0.41}$	$14.26_{\pm 0.65}$
SPECTER	$58.00_{\pm 0.66}$	$40.44_{\pm 1.17}$	$42.81_{\pm 0.53}$	$70.15_{\pm 0.67}$	$\mathbf{69.82}_{\pm 1.25}$	$58.99_{\pm 0.82}$	$63.36_{\pm 0.36}$	$48.66_{\pm 0.14}$	$58.96_{\pm 0.23}$
GIANT	$58.00_{\pm 0.82}$	$39.69_{\pm 1.22}$	$43.73_{\pm 0.68}$	$61.99_{\pm 0.78}$	$47.60_{\pm 4.18}$	$47.51_{\pm 1.14}$	$63.06_{\pm 0.53}$	$48.57_{\pm 0.89}$	$58.68_{\pm 0.25}$
GRENADE	$\mathbf{61.96}_{\pm 0.79}$	$\mathbf{44.98}_{\pm 1.85}$	$\mathbf{49.19}_{\pm 0.63}$	$\mathbf{73.54}_{\pm 0.75}$	$69.64_{\pm 1.64}$	$\mathbf{64.14}_{\pm 0.71}$	$\mathbf{64.89}_{\pm 0.30}$	$\mathbf{50.22}_{\pm 0.42}$	$\mathbf{59.68}_{\pm 0.23}$

Supervised Node Classification

Methods	arxiv MLP	arxiv GraphSAGE	arxiv RevGAT-KD	products MLP	products GraphSAGE	citation2 MLP	citation2 GraphSAGE
OGB	$55.50_{\pm 0.23}{}^{\star}$	$71.49_{\pm 0.27}{}^{\star}$	$74.26_{\pm 0.17}{}^{\star}$	$61.06_{\pm 0.08}{}^{\star}$	$75.81_{\pm 0.46}$	$48.98_{\pm 1.74}$	$62.10_{\pm 0.25}$
BERT	$62.91_{\pm 0.60}{}^{\star}$	$70.97_{\pm 0.33}{}^{\star}$	$73.59_{\pm 0.10}{}^{\star}$	$60.90_{\pm 1.09}{}^{\star}$	$80.70_{\pm 0.50}$	$56.75_{\pm 0.33}$	$60.38_{\pm 0.67}$
BERT+MLM	$67.71_{\pm 0.22}$	$73.65_{\pm 0.14}$	$75.39_{\pm 0.16}$	$76.86_{\pm 0.24}$	$80.90_{\pm 0.11}$	$66.11_{\pm 0.35}$	$64.57_{\pm 0.50}$
SimCSE	$60.58_{\pm 0.13}$	$67.26_{\pm 0.24}$	$73.69_{\pm 0.15}$	$67.69_{\pm 0.06}$	$80.41_{\pm 0.44}$	$53.91_{\pm 0.36}$	$58.75_{\pm 0.24}$
SPECTER	$70.40_{\pm 0.25}$	$74.19_{\pm 0.18}$	$75.61_{\pm 0.67}$	$75.38_{\pm 0.22}$	$79.42_{\pm 0.34}$	$54.20_{\pm 0.67}$	$66.58_{\pm 0.23}$
GIANT	$73.08_{\pm 0.06}{}^{\star}$	$74.59_{\pm 0.28}{}^{\star}$	$76.12_{\pm 0.16}{}^{\star}$	$79.82_{\pm 0.07}{}^{\star}$	$82.03_{\pm 0.65}$	$67.24_{\pm 0.27}$	$70.32_{\pm 0.27}$
GLEM	-	$73.59_{\pm 0.40}$	-	-	$82.02_{\pm 0.62}$	-	$68.25_{\pm 0.18}$
GRENADE	$\mathbf{73.16}_{\pm 0.12}$	$\mathbf{75.00}_{\pm 0.19}$	$\mathbf{76.21}_{\pm 0.17}$	$\mathbf{81.58}_{\pm 0.18}$	$\mathbf{83.11}_{\pm 0.56}$	$\mathbf{68.11}_{\pm 0.34}$	$\mathbf{70.89}_{\pm 0.34}$

Grenade: Graph-Centric Language Model for Self-Supervised Representation Learning on Text-Attributed Graphs

未来展望

1. **LLM用于多模态图。**节点可能包含来自多种模态的特征，通过开发可以处理多模态数据的LLMs，可以对图结构进行更准确和更全面的推理，不仅考虑文本信息，还考虑视觉、听觉和其他类型的数据。
2. **效率和更少的计算成本。**LLM在推理和计算阶段的成本阻碍了他们处理大规模图的能力，LLM与GNN集成时，两个模型的融合也会越来越困难。随着图尺寸的增加，输入序列的长度会显著增加，二大模型中较长的输入序列将导致更高的时间和内存复杂度。因此，发现和实施有效的策略来训练 LLM 和 GNN 并降低计算成本变得至关重要。
3. **处理不同的图任务。**LLM卓越的能力能够处理更复杂或是生成式的任务，包括但不限于图生成、图理解和图问答。通过扩展基于LLM的方法可以涵盖这些复杂的任务。在药物发现领域，LLM可以促进新型分子结构的生成；在社交网络分析中，可以提供对复杂关系模式的更深入的见解；在知识图谱构建中，可以有助于创建更全面、更准确的知识库。
4. **以用户为中心的图智能体。**目前的图智能体主要是针对单独的图任务量身定制的，未来的图智能体方向应该致力于以用户为中心，具有在图数据中动态搜索答案的能力，并且具备多次交互式运行的功能，以响应用户提出的各种开放式问题。

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I am currently an associate professor at Mila-Quebec AI Institute and HEC Montreal. Prior to that, I was a Postdoc at University of Michigan and Carnegie Mellon University. I also worked at Microsoft Research Asia as an associate researcher between 2014-2016. For more information, please check my CV.

Hiring!! Our group has multiple PhD positions next Fall. In particular, we are looking for students to work on the following projects:

- Geometric Deep Learning, Graph Neural Networks for Drug Design
- Equivariant Neural Networks for Molecular Simulation
- Knowledge Graph Construction and Reasoning, Natural Language Understanding

Mila魁北克人工智能研究院 唐建

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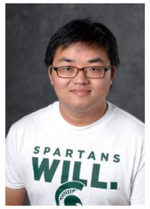

Jiliang Tang is a University Foundation Professor in the computer science and engineering department at Michigan State University. He got one early promotion to associate professor at 2021 and then a promotion to full professor (designated as MSU foundation professor) at 2022. Before that, he was a research scientist in Yahoo Research and got his PhD from Arizona State University in 2015 under Dr. Huan Liu. His research interests include graph machine learning,trustworthy AI and their applications in education and biology. He was the recipient of various awards including 2022 AI's 10 to Watch, 2022 IAPR J. K. AGGARWAL Award, 2022 SIAM/IBM Early Career Research Award, 2021 IEEE ICDM Tao Li Award, 2021 IEEE Big Data Security Junior Research Award, 2020 ACM SIGKDD Rising Star Award, 2020 Distinguished Withrow Research Award, 2019 NSF Career Award, and 8 best paper awards (or runner-ups). His dissertation won the 2015 KDD Best Dissertation runner up and Dean's Dissertation Award. He serves as conference organizers (e.g., KDD, SIGIR, WSDM and SDM) and journal editors (e.g., TKDD, TOIS and TKDE). He has published his research in highly ranked journals and top conference proceedings, which have received tens of thousands of citations with h-index 95 (Google Scholar) and extensive media coverage (Links).

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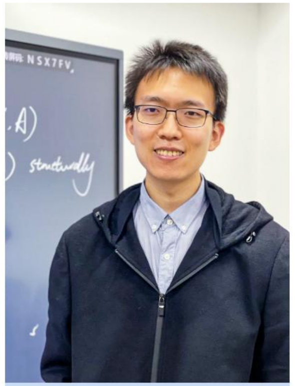

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Biography

Muhan is a tenure-track assistant professor and PhD advisor in the Institute for Artificial Intelligence of Peking University . Before coming back to China, he was a research scientist in Facebook AI (now Meta AI) working on large-scale graph learning systems and problems (2019-2021). He received his PhD degree in computer science from Washington University in St. Louis (2015-2019), advised by Prof. Yixin Chen. Before WashU, he obtained a bachelor degree from Shanghai Jiao Tong University as a member of the IEEE pilot class, where he worked with Prof. Ya Zhang and Prof. Wenjun Zhang.

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