Towards Graph Foundation Models

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Outline

- Background
- Graph Foundation Model
- Our Recent Attempts
- Future Directions

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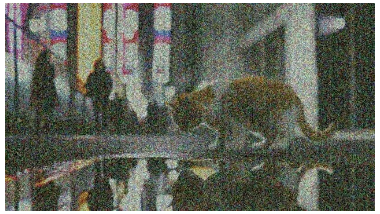
- Future Directions

Foundation Models

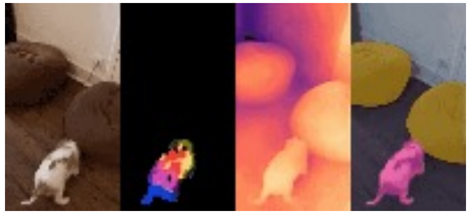
“A foundation model is any model that is trained on broad data and can be adapted to a wide range of downstream tasks.” [1]

Language



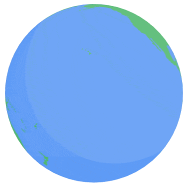
OpenAI × GPT4

Vision



Meta × DINOv2

Speech



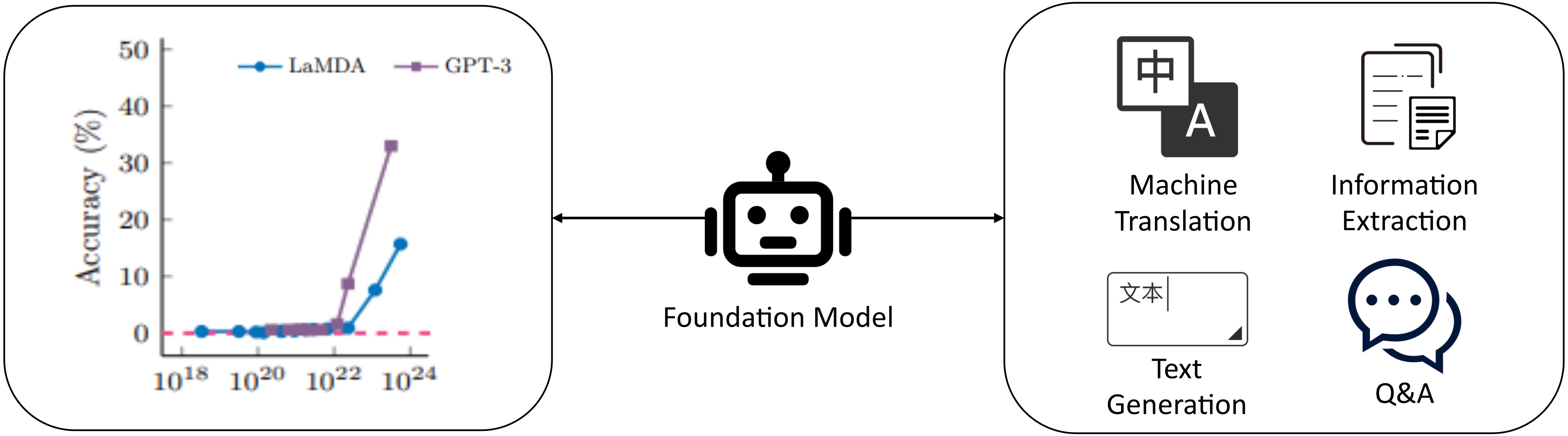
Google × USM

Foundation models have become a reality in language, vision, and speech.

[1] R. Bommasani, D. A. Hudson, E. Adeli, R. Altman, S. Arora, S. von Arx, M. S. Bernstein, J. Bohg, A. Bosselut, E. Brun-skill, et al., “On the opportunities and risks of foundation models,” arXiv preprint arXiv:2108.07258, 2021

Characteristics of Foundation Models

- Emergence suggests that as a foundation model scales up, it may spontaneously manifest novel capabilities. [2]
- Homogenization alludes to the model's versatility, enabling its deployment across diverse applications.



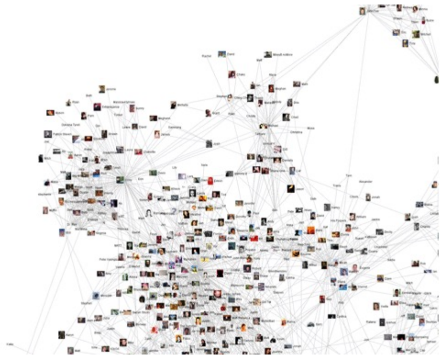
Emergence

Homogenization

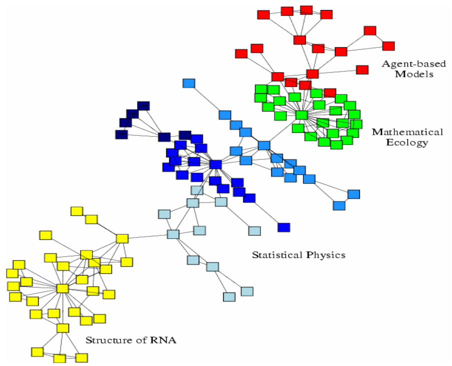
[2] Wei J, Tay Y, Bommasani R, et al. Emergent abilities of large language models[J]. arXiv preprint arXiv:2206.07682, 2022.

On the other hand…

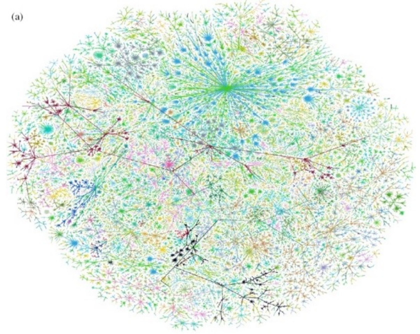
Graph (network) is a common language for describing relational data.



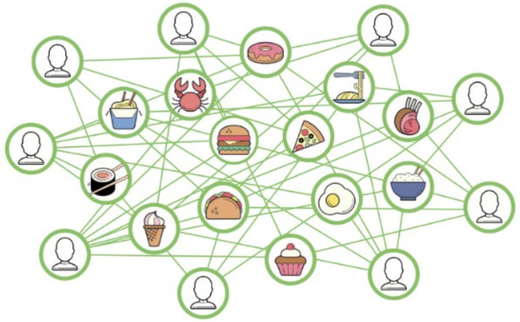
Social Network



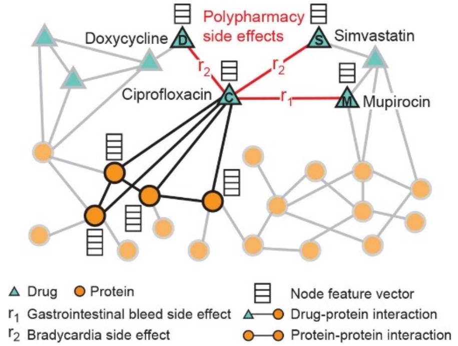
Citation Network



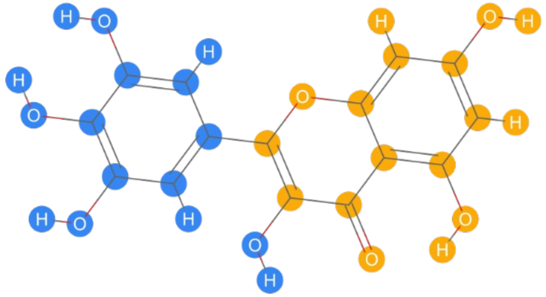
Internet



User-item Graph

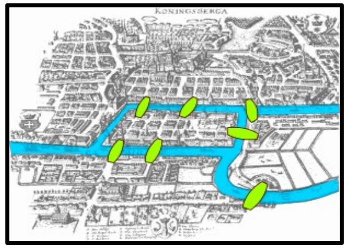


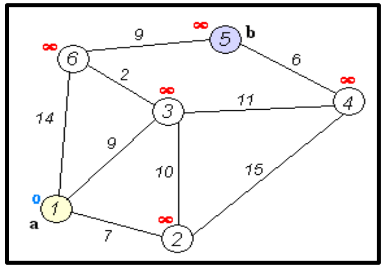
Drug Interaction Graph

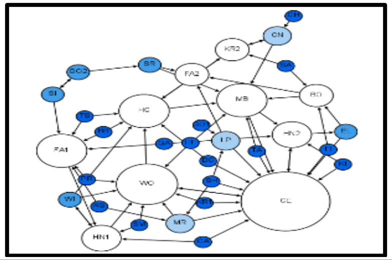


Molecule Graph

A History of Graph Theory & Learning







Graph Theory
- Euler’s seven bridges

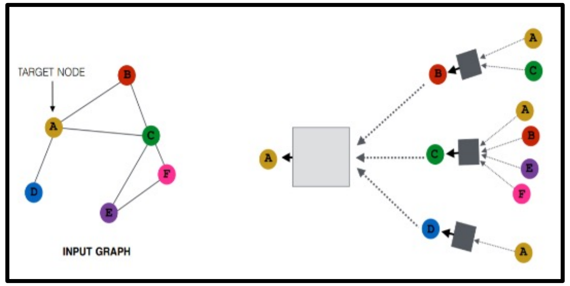
Graph Algorithm
- Dijkstra's shortest path

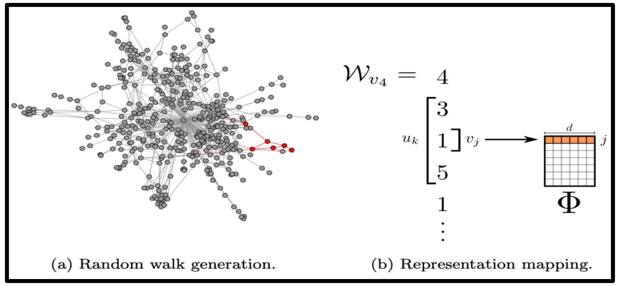
Graph Models
- Random graph, Stochastic block model, Scale-free network…

1736 → 1950s → 1990s → 2000s → 2010s → 2020s

Graph Neural Network
- GCN, GAT…

Graph Embedding
- Laplacian Eigenmap, DeepWalk…





Outline

- Background
- Graph Foundation Model
- Our Recent Attempts
- Summary

What'll be the Next Paradigm of Graph Learning?

A survey discussing the potential future of graph learning

Towards Graph Foundation Models: A Survey and Beyond

Jiawei Liu*, Cheng Yang*, Zhiyuan Lu, Junze Chen, Yibo Li, Meng-mei Zhang, Ting Bai, Yuan Fang, Lichao Sun, Philip S. Yu, and Chuan Shi

Abstract—Emerging as fundamental building blocks for diverse artificial intelligence applications, foundation models have achieved notable success across natural language processing and many other domains. Parallelly, graph machine learning has witnessed a transformative shift, with shallow methods giving way to deep learning approaches. The emergence and homogenization capabilities of foundation models have piqued the interest of graph machine learning researchers, sparking discussions about developing the next graph learning paradigm that is pre-trained on broad graph data and can be adapted to a wide range of downstream graph tasks. However, there is currently no clear definition and systematic analysis for this type of work. In this article, we propose the concept of graph foundation models (GFMs), and provide the first comprehensive elucidation on their key characteristics and technologies. Following that, we categorize existing works towards GFMs into three categories based on their reliance on graph neural networks and large language models. Beyond providing a comprehensive overview of the current landscape of graph foundation models, this article also discusses potential research directions for this evolving field.

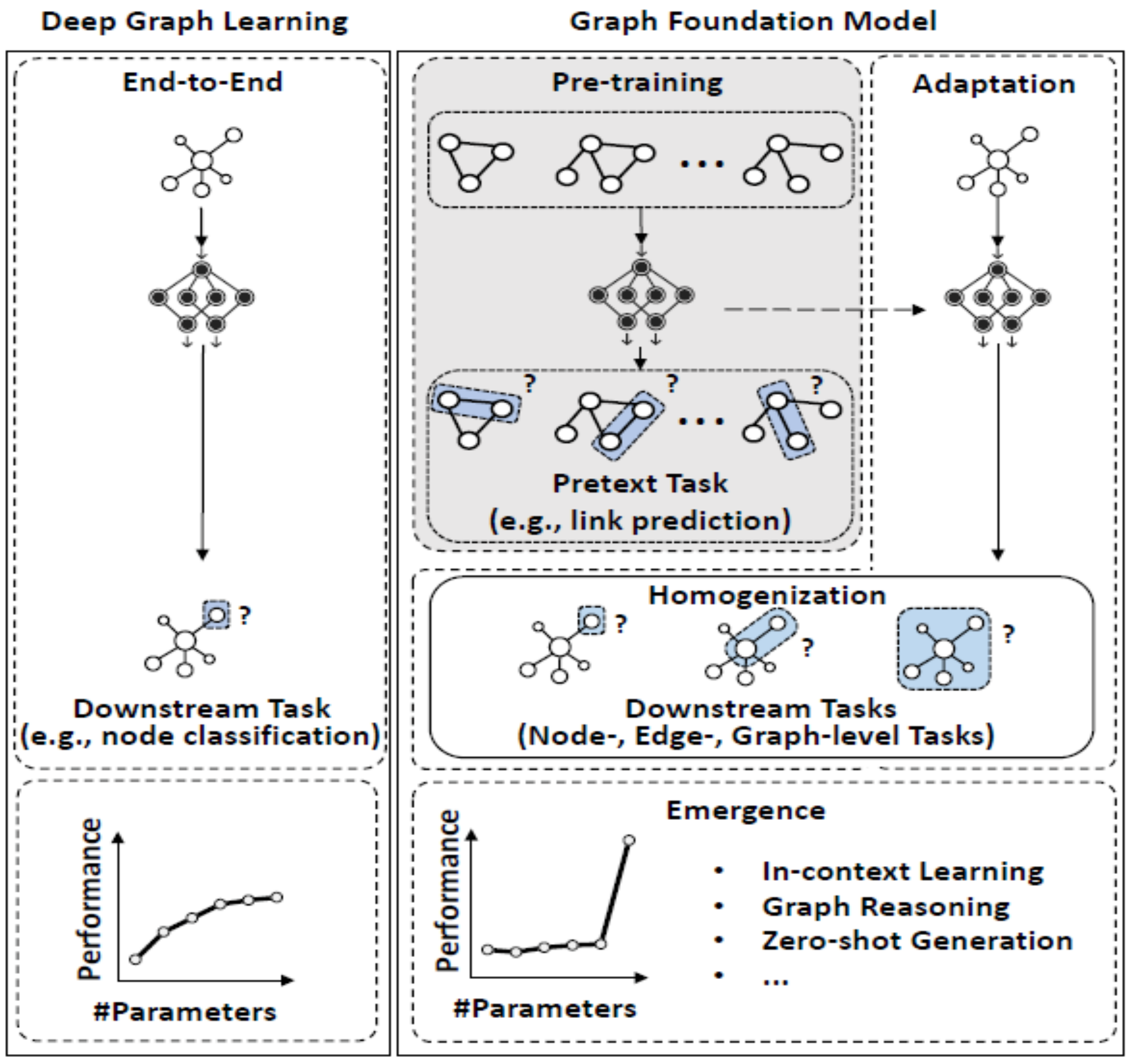
Jiawei Liu, Cheng Yang, Zhiyuan Lu, Junze Chen, Yibo Li, Mengmei Zhang, Ting Bai, Yuan Fang, Lichao Sun, Philip S. Yu, Chuan Shi. Towards Graph Foundation Models: A Survey and Beyond. arXiv 2023

Graph Foundation Model (GFM)

A GFM is envisioned as a model pre-trained on extensive graph data, primed for adaptation across diverse downstream graph tasks.

Two expected characteristics：

- Emergence refers to novel capabilities shown exclusively in large-scale graph models.
- Homogenization denotes the adaptability across different types of graph tasks.



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Relationship with Language Foundation Model

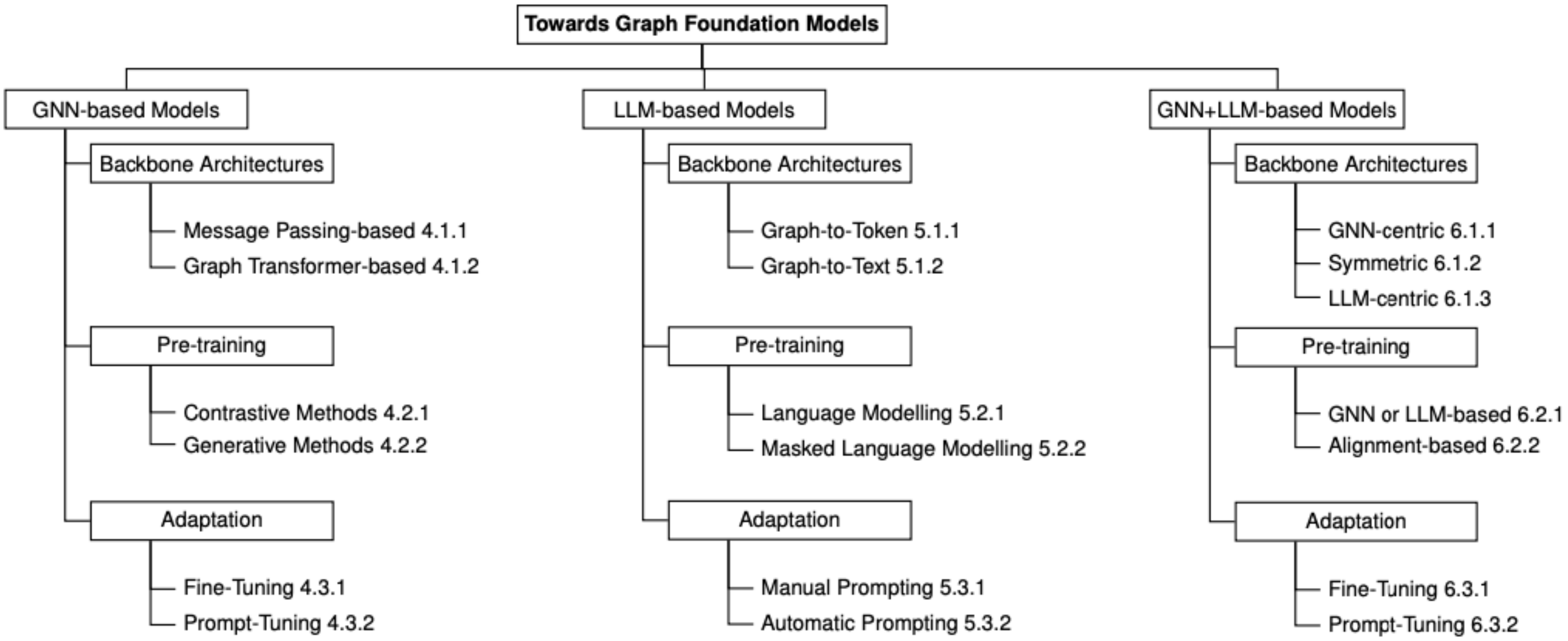
Similarities & Differences

		Language Foundation Model	Graph Foundation Model
Similarities	Goal	Enhancing the model's expressive power and its generalization across various tasks	
	Paradigm	Pre-training and Adaptation	
Intrinsic differences	Data	Euclidean data (text)	Non-Euclidean data (graphs) or a mixture of Euclidean (e.g., graph attributes) and non-Euclidean data
	Task	Similar formats	Diverse formats
Extrinsic differences	Backbone Architectures	Mostly based on Transformer	No unified architecture
	Homogenization	Easy to homogenize	Difficult to homogenize
	Domain Generalization	Strong generalization capability	Weak generalization across datasets
	Emergence	Has demonstrated emergent abilities	No/unclear emergent abilities as of the time of writing

Existing Work towards GFMs

No clear solution of how to build a GFM yet ☹

But there are some explorations towards it ☺



GNN-based Models

Idea: Improve existing graph learning through innovation in GNN

- Backbone
- Pre-training
- Adaptation

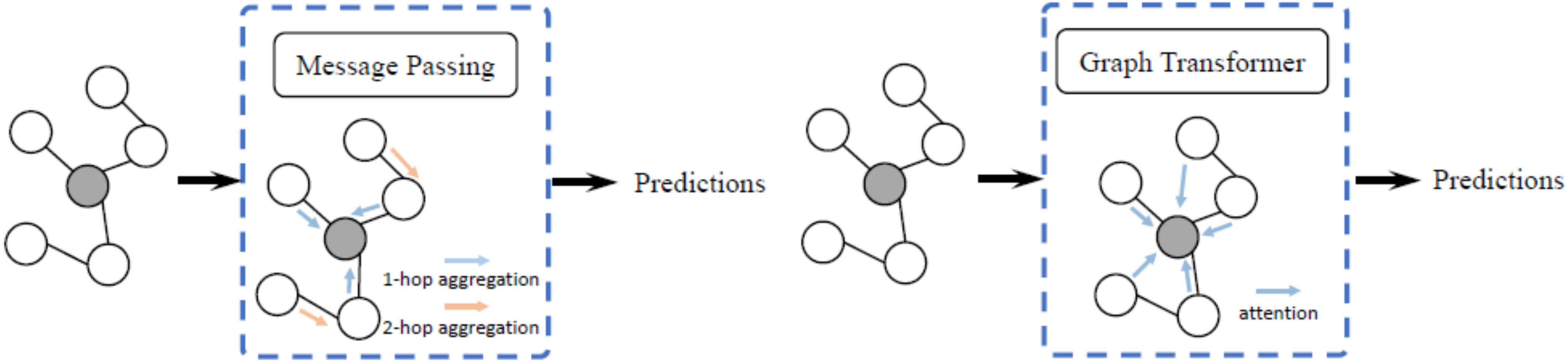
These works typically

- draw inspiration from the model architectures or training paradigms used in NLP
- do not explicitly model text data in their pipeline

GNN-based Models

Backbone Architecture

- Message Passing
- Graph Transformer

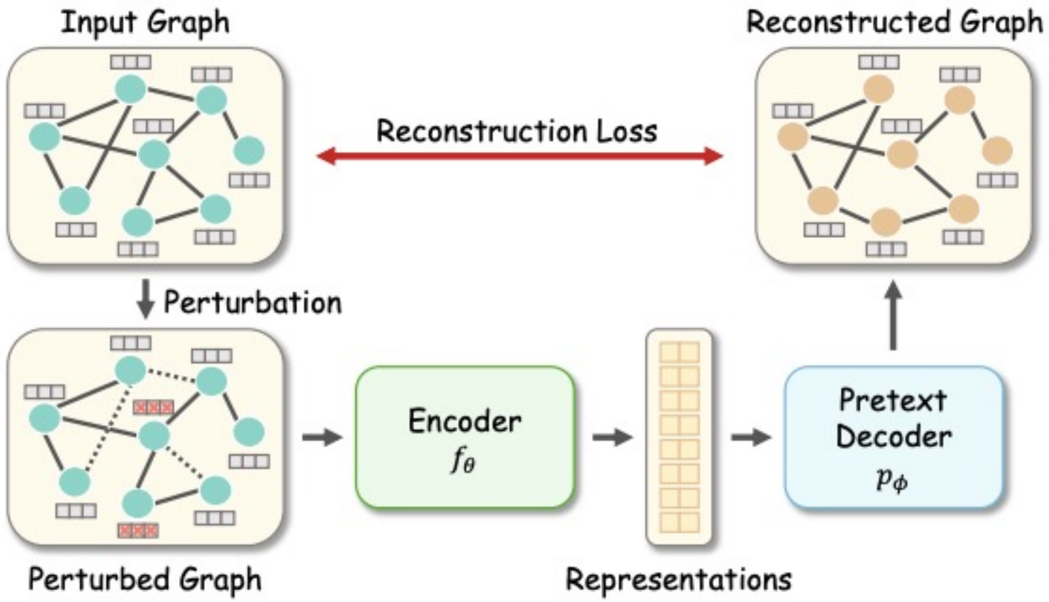


(a) Message Passing. (b) Graph Transformer.

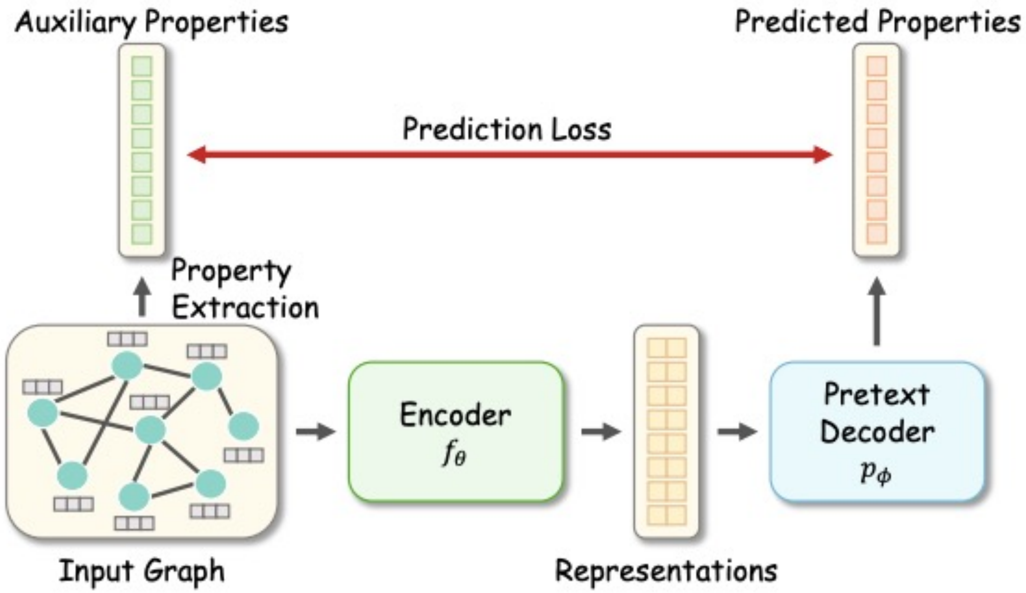
GNN-based Models

Pre-training

- Generative methods: graph reconstruction, property prediction
- Contrastive methods: same-scale contrastive learning, cross-scale contrastive learning



graph reconstruction



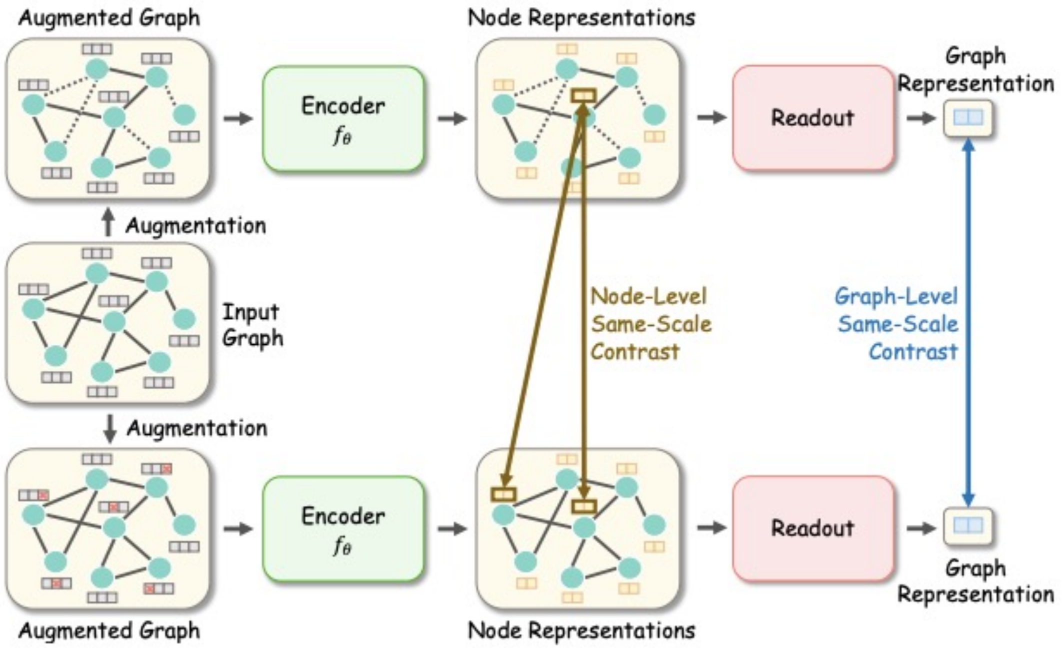
property prediction

Liu Y, Jin M, Pan S, et al. Graph self-supervised learning: A survey[J]. IEEE Transactions on Knowledge and Data Engineering, 2022, 35(6): 5879-5900.

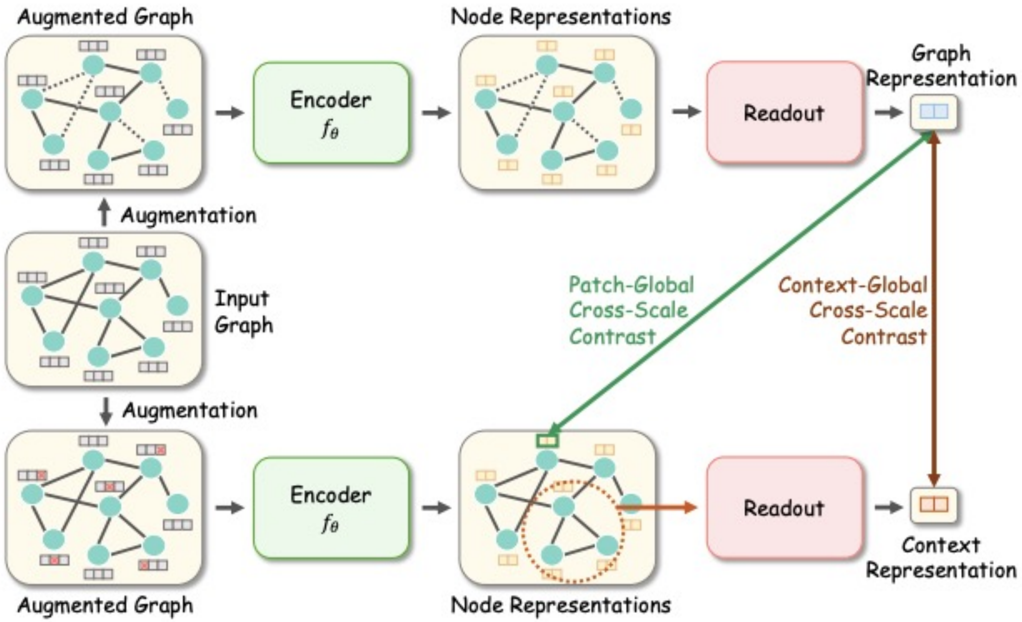
GNN-based Models

Pre-training

- Generative methods: graph reconstruction, property prediction
- Contrastive methods: same-scale contrastive learning, cross-scale contrastive learning



same-scale contrastive learning



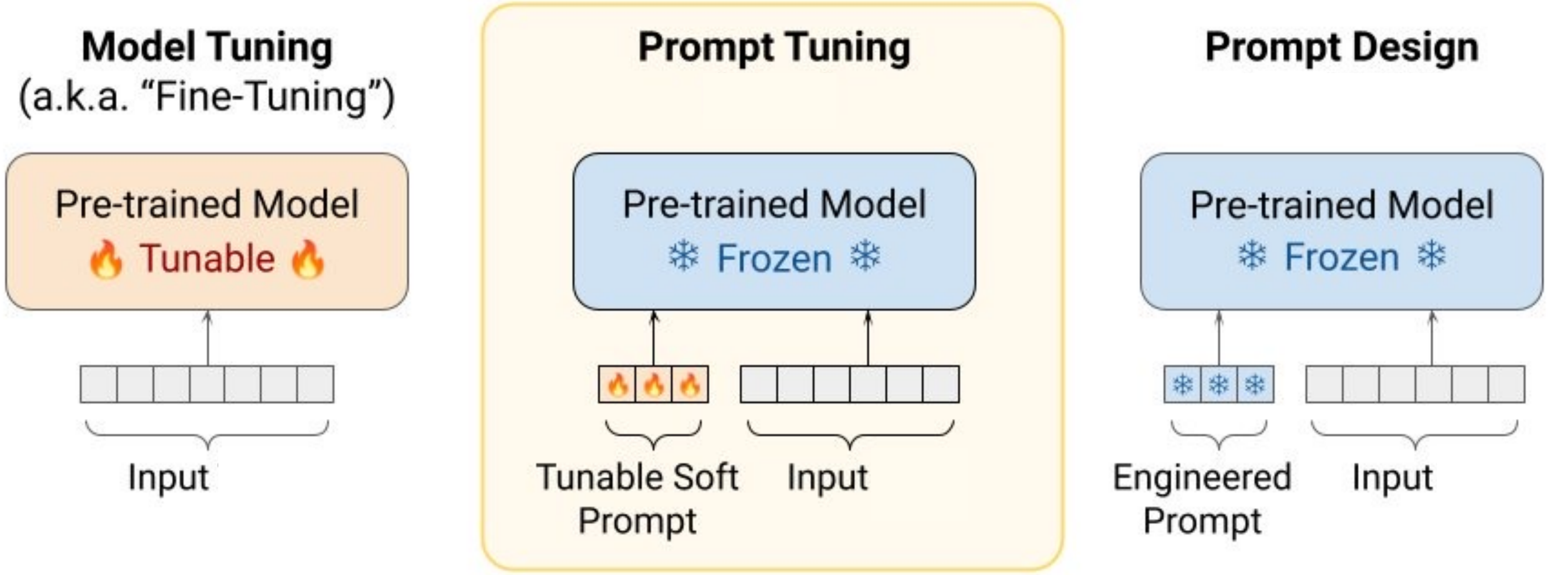
cross-scale contrastive learning

Liu Y, Jin M, Pan S, et al. Graph self-supervised learning: A survey[J]. IEEE Transactions on Knowledge and Data Engineering, 2022, 35(6): 5879-5900.

GNN-based Models

Adaptation

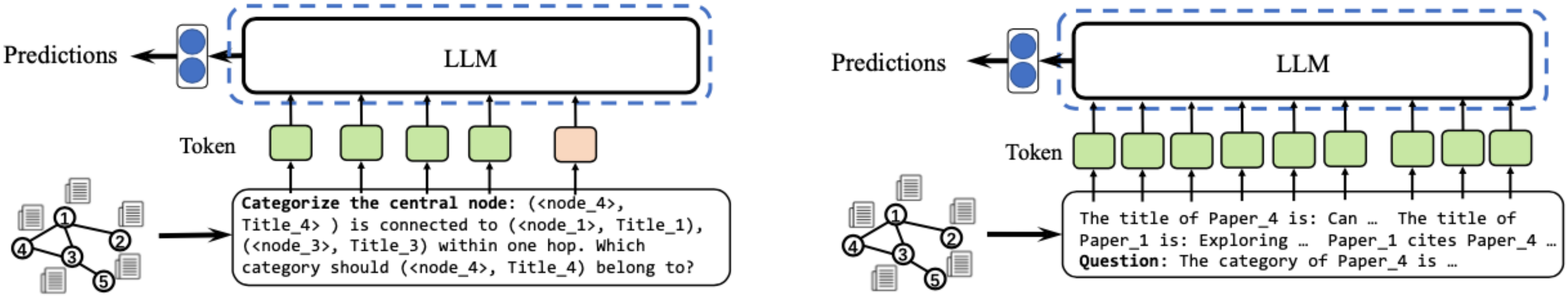
- Fine-tuning: keep input graph intact, modify model parameters accordingly
- Prompt-tuning: keep pre-trained model intact, modify input graph instead



LLM-based Models

Idea: Exploring the feasibility of using LLMs as GFMs by serializing graphs

- Graph-to-token: describe graph structure with token sequence
- Graph-to-text: describe graph information with natural language



(a) Graph-to-token. (b) Graph-to-text.

LLM-based Models

Brief Summary of Existing Work

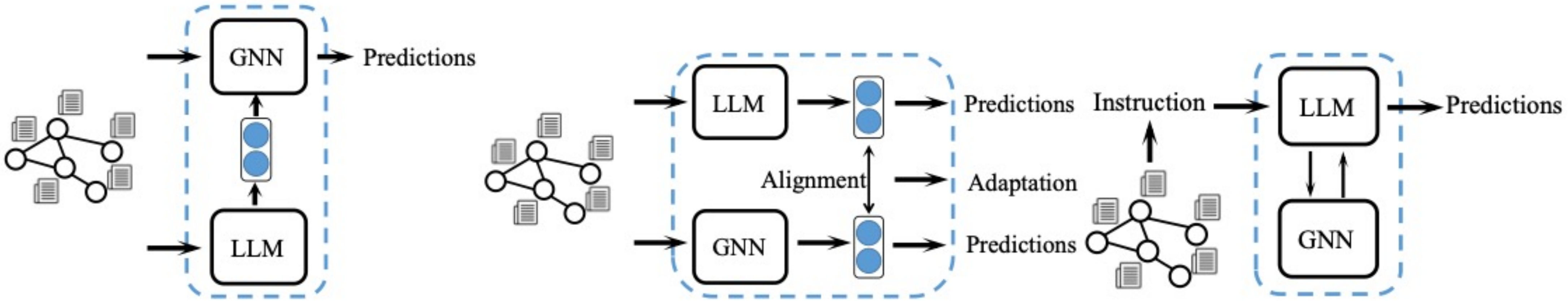
- Backbone: BERT, T5, LLaMa, GPTs…
- Pre-training: Language Model (LM), Masked Language Model (MLM)
- Adaptation: Manual Prompt Tuning, Automatic Prompt Tuning

Model	Backbone Architecture			Pre-training	Adaptation
InstructGLM[157]	Graph-to-token	+	Flan-T5/LLaMA	MLM,LM	Manual Prompt Tuning
LLMtoGraph[71]	Graph-to-text	+	GPTs, Vicuna	LM	Manual Prompt Tuning
NLGraph[126]	Graph-to-text	+	GPTs	LM	Manual Prompt Tuning
GraphText[175]	Graph-to-text	+	GPTs	LM	Manual Prompt Tuning
LLM4Mol[91]	Graph-to-text	+	GPTs	LM	Manual Prompt Tuning
GPT4Graph[29]	Graph-to-text	+	GPT-3	LM	Manual Prompt Tuning + Automatic Prompt Tuning
Graph-LLM[9]	Graph-to-text	+	BERT, DeBERTa, Sentence-BERT, GPTs, LLaMA	MLM,LM	Manual Prompt Tuning + Automatic Prompt Tuning

GNN+LLM-based Models

Idea: Harness the strengths of both language understanding from LLMs and structural analysis from GNNs

- GNN-centric: utilize LLMs to extract features from raw data and predict with GNNs
- Symmetric: align the embeddings of GNNs and LLMs to make better predictions
- LLM-centric: utilize GNNs as tools to enhance the performance of LLM



(a) GNN-centric methods. (b) Symmetric methods. (c) LLM-centric methods.

GNN+LLM-based Models

Brief Summary of Existing Work

- Backbone: GNN-centric, Symmetric, LLM-centric
- Pre-training: LM, MLM, Graph-Text Contrastive Learning (GTCL)…
- Adaptation: (Parameter-Efficient) Fine-tuning, Tuning-free Prompting, Prompt Tuning

Model	Backbone Architecture	Pre-training	Adaptation
SimTeG [16]	GNN-centric	MLM, TTCL	Parameter-Efficient FT
TAPE [35]	GNN-centric	LM	Tuning-free Prompting + Parameter-Efficient FT
GIANT [11]	GNN-centric	MLM	Vanilla FT
GraD [79]	GNN-centric	MLM	Parameter-Efficient FT
GraphFormer [153]	Symmetric	MLM	Vanilla FT
GLEM [174]	Symmetric	MLM	Vanilla FT
ConGrat [4]	Symmetric	MLM + GTCL	Parameter-Efficient FT
G2P2 [136]	Symmetric	GTCL	Prompt Tuning
SAFER [6]	Symmetric	MLM	Parameter-Efficient FT
Text2Mol [18]	Symmetric	MLM + GTCL	Parameter-Efficient FT
MoMu [109]	Symmetric	MLM + GTCL	Parameter-Efficient FT
MoleculeSTM [73]	Symmetric	MLM + GTCL	Parameter-Efficient FT
CLAMP [103]	Symmetric	MLM + GTCL	Parameter-Efficient FT
Graph-Toolformer [165]	LLM-centric	LM	Tuning-free Prompting + Vanilla FT

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Our Recent Attempts

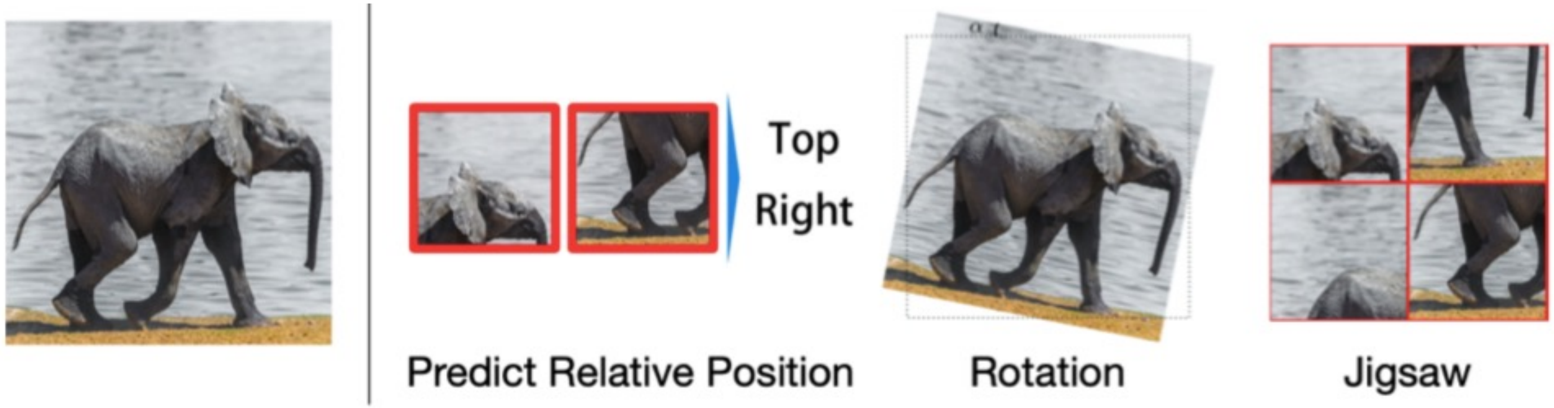
- MA-GCL: Model Augmentation Tricks for Graph Contrastive Learning (MA-GCL, AAAI 2023)
- A Data-centric Framework to Endow Graph Neural Networks with Out-Of-Distribution Detection Ability   (AAGOD, KDD 2023)
- GraphTranslator: Aligning Graph Model to Large Language Model for Open-ended Tasks (GraphTranslator, WWW 2024)

Xumeng Gong, Cheng Yang, Chuan Shi. MA-GCL: Model Augmentation Tricks for Graph Contrastive Learning. AAAI 2023
Yuxin Guo, Cheng Yang, Yuluo Chen, Jixi Liu, Chuan Shi, Junping Du. A Data-centric Framework to Endow Graph Neural Networks with Out-Of-Distribution Detection Ability. KDD 2023
Mengmei Zhang, Mingwei Sun, Peng Wang, Shen Fan, Yanhu Mo, Xiaoxiao Xu, Hong Liu, Cheng Yang, Chuan Shi. GraphTranslator: Aligning Graph Model to Large Language Model for Open-ended Tasks. WWW 2024

Motivation of MA-GCL

Motivation

- Contrastive learning captures invariant information among different augmentation views.
- Good augmentations should introduce as much perturbation as possible without changing the core semantics.



- However, in graph contrastive learning (GCL), we have few prior knowledge on how to generate such good augmentations.

Can we generate better augmentations than typical random dropping-based methods?

MAGCL

Core idea

- We interpret a GNN as a sequence of propagation operator *g* and transformation operator *h*:
  - propagation operator *g* is typically the non-parametric graph filter.
  - transformation operator *h* is typically a weight matrix with a non-linear function.

$$g(\boldsymbol{Z};\boldsymbol{F}) = \boldsymbol{F}\boldsymbol{Z},\ h(\boldsymbol{Z};\boldsymbol{W}) = \sigma(\boldsymbol{Z}\boldsymbol{W}), \qquad \boldsymbol{F} = \boldsymbol{D}^{-\frac{1}{2}}\boldsymbol{A}\boldsymbol{D}^{-\frac{1}{2}}$$

$$GCN(\boldsymbol{X}) = h_L \circ g \circ h_{L-1} \circ g \circ \cdots \circ h_1 \circ g(\boldsymbol{X}),$$

$$SGC(\boldsymbol{X}) = h \circ g^{[L]}(\boldsymbol{X}),$$

- Intuition: different architectures (i.e., operator sequences) won't affect the core semantics.
- Thus we perturb the neural architecture of graph encoder as model augmentations.

MAGCL

We propose three strategies to introduce perturbations:

- Asymmetric strategy
  - Use the same number of operator *h* with shared parameters for different views
  - Use different numbers of operator *g* for different views
- Random strategy
  - Randomly vary the number of propagation operator *g* in every training epoch
- Shuffling strategy
  - Randomly shuffle the permutation of propagation and transformation operators

Experiments

We conducted extensive experiments on node/graph classification/clustering.

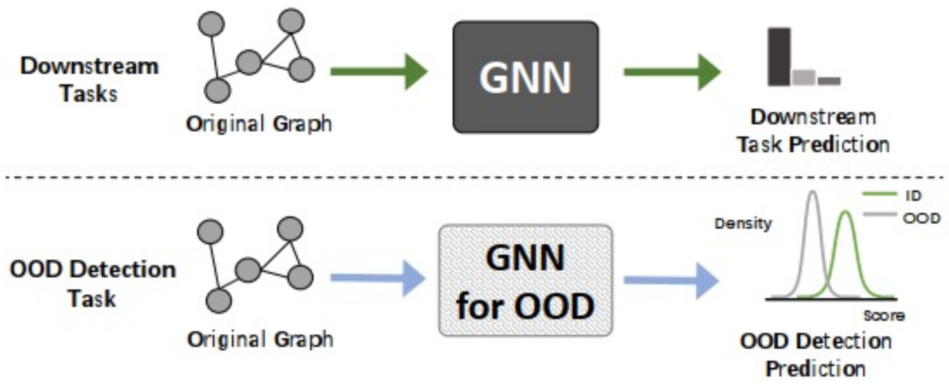
Datasets	Cora	CiteSeer	PubMed	Coauthor-CS	Amazon-C	Amazon-P	Avg. Acc.	Avg. Rank
GCN	82.5 ± 0.4	71.2 ± 0.3	79.2 ± 0.3	93.03 ± 0.3	86.51 ± 0.5	92.42 ± 0.2		
GAT	83.0 ± 0.7	72.5 ± 0.7	79.0 ± 0.3	92.31 ± 0.2	86.93 ± 0.3	92.56 ± 0.4	-	-
InfoGCL	83.5 ± 0.3	73.5 ± 0.4	79.1 ± 0.2	-	-	-		
DGI	82.3 ± 0.6	71.8 ± 0.7	76.8 ± 0.3	92.15 ± 0.6	83.95 ± 0.5	91.61 ± 0.2	83.10	8.5
GRACE	81.7 ± 0.4	71.5 ± 0.5	80.7 ± 0.4	92.93 ± 0.0	87.46 ± 0.2	92.15 ± 0.2	84.44	6.5
MVGRL	83.4 ± 0.3	73.0 ± 0.3	80.1 ± 0.6	92.11 ± 0.1	87.52 ± 0.1	91.74 ± 0.0	84.63	6.5
BGRL	81.7 ± 0.5	72.1 ± 0.5	80.2 ± 0.4	93.01 ± 0.2	88.23 ± 0.3	92.57 ± 0.3	84.63	6.5
GCA	83.4 ± 0.3	72.3 ± 0.1	80.2 ± 0.4	93.10 ± 0.0	87.85 ± 0.3	92.53 ± 0.2	84.89	4.0
SimGRACE	77.3 ± 0.1	71.4 ± 0.1	78.3 ± 0.3	93.45 ± 0.4	86.04 ± 0.2	91.39 ± 0.4	82.98	8.5
COLES	81.2 ± 0.4	71.5 ± 0.2	80.4 ± 0.7	92.65 ± 0.1	79.64 ± 0.0	89.00 ± 0.5	82.40	8.8
ARIEL	82.5 ± 0.1	72.2 ± 0.2	80.5 ± 0.3	93.35 ± 0.0	88.27 ± 0.2	91.43 ± 0.2	84.71	4.8
CCA-SSG	**83.9 ± 0.4**	73.1 ± 0.3	81.3 ± 0.4	93.37 ± 0.2	88.42 ± 0.3	92.44 ± 0.1	85.42	2.3
Base Model	81.1 ± 0.4	71.4 ± 0.1	79.1 ± 0.4	92.86 ± 0.3	87.65 ± 0.2	91.19 ± 0.3	83.88	9.0
MA-GCL	83.3 ± 0.4	**73.6 ± 0.1**	**83.5 ± 0.4**	**94.19 ± 0.1**	**88.83 ± 0.3**	**93.80 ± 0.1**	**86.20**	**1.2**

Motivation of AAGOD

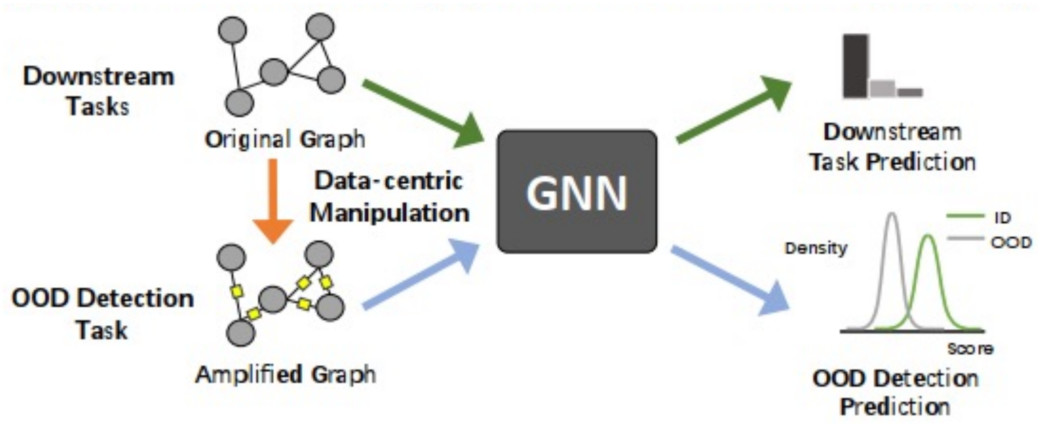
Motivation

- A reliable GNN should not only perform well on know samples (ID) but also identify graphs it has not been exposed to before (OOD) .
- Existing works proposes to train a neural network specialized for the OOD detection task.

Can we build a graph prompt that can solve OOD detection given a well-trained GNN?



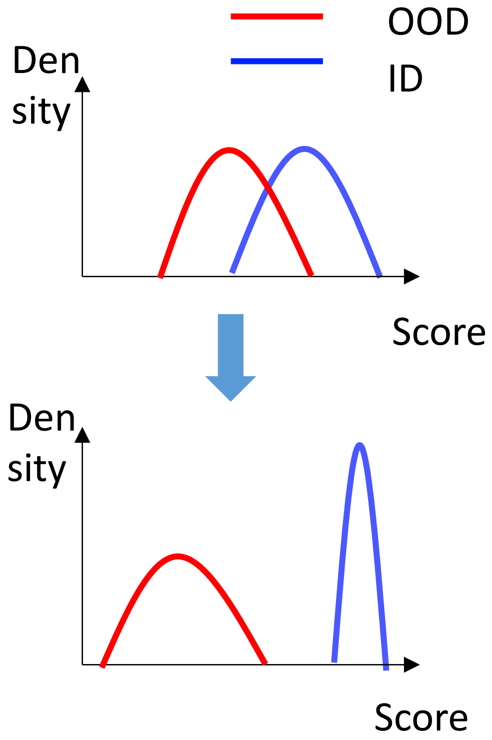
(1) Traditional works

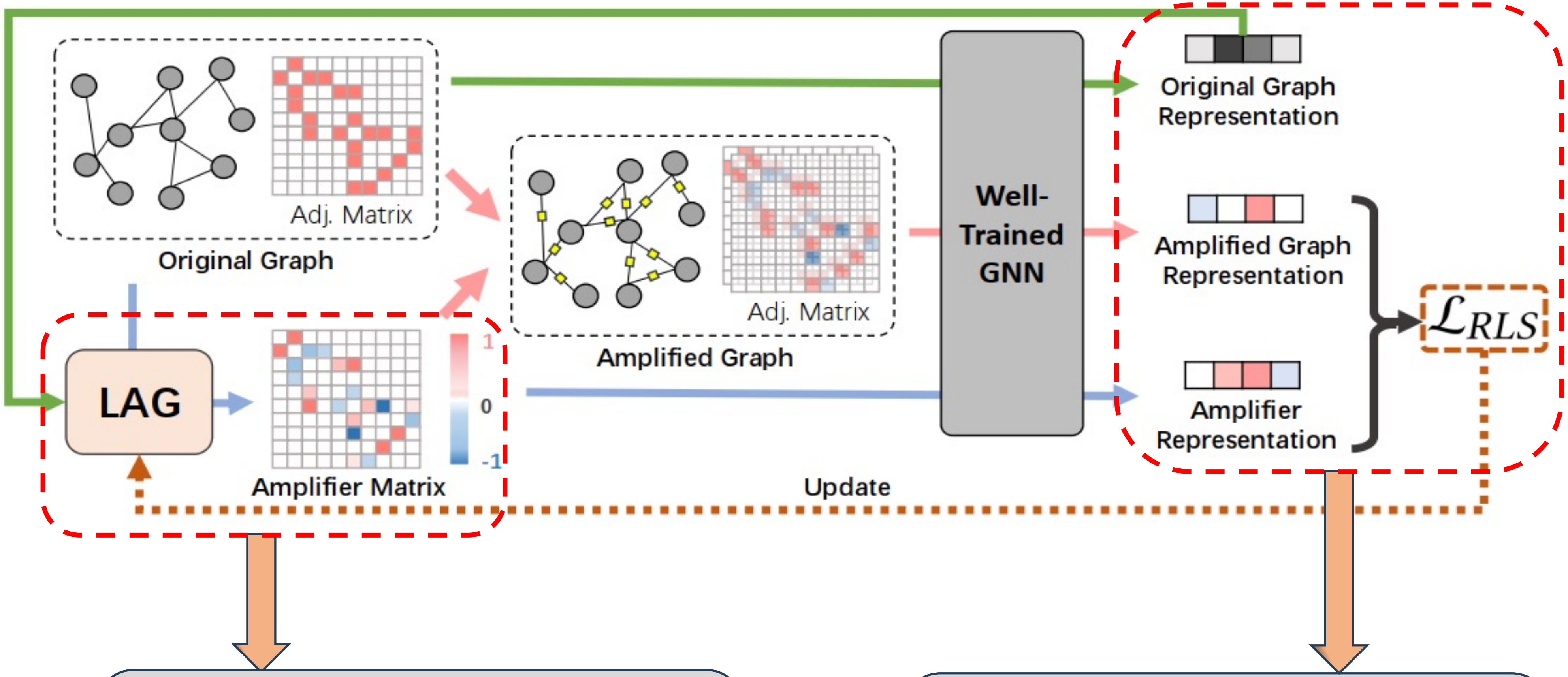


(2) Our proposed framework

AAGOD

We modify edge weights as prompts to highlight the latent pattern of ID graphs, and thus enlarge the score gap between OOD and ID graphs.





LAG adaptively generates graph-specific amplifiers by converting node representations into edge weights.

RLS encourages high scores for amplified ID graphs and expects low scores when only seeing the amplifiers.

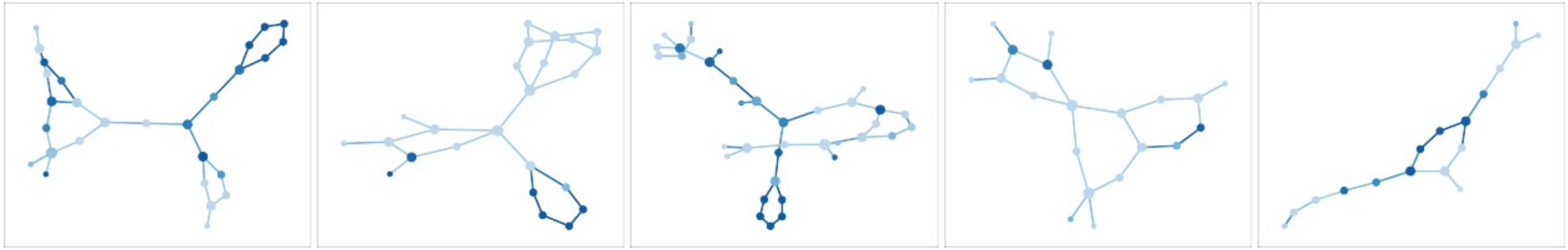
Experiments

We conducted experiments on five dataset pairs over four GNNs to verify performance.

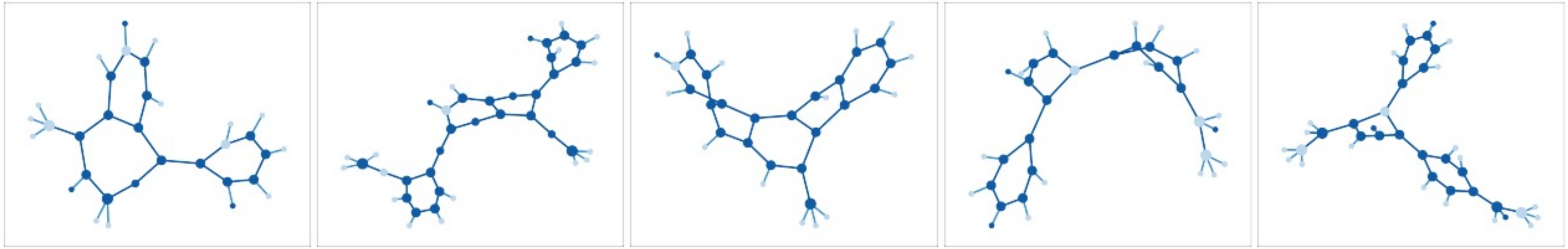
ID	OOD	Metric	GCL_S	GCL_S+	Improv.	GCL_L	GCL_L+	Improv.	$JOAO_S$	$JOAO_S$+	Improv.	$JOAO_L$	$JOAO_L$+	Improv.
ENZYMES	PROTEIN	AUC ↑	62.97	**73.76**	+17.14%	62.56	**67.15**	+7.34%	61.20	**74.19**	+21.23%	59.68	**65.11**	+9.10%
		AUPR ↑	62.47	**75.27**	+20.49%	**65.45**	65.18	-0.41%	61.30	**77.10**	+25.77%	64.16	**64.49**	+0.51%
		FPR95 ↓	93.33	**88.33**	-5.36%	93.30	**85.00**	-8.90%	90.00	**81.67**	-9.26%	96.67	**85.00**	-12.07%
IMDBM	IMDBB	AUC ↑	80.52	**83.84**	+4.12%	61.08	**68.64**	+12.38%	80.40	**82.80**	+2.99%	48.25	**64.32**	+33.31%
		AUPR ↑	74.43	**80.16**	+7.70%	59.52	**68.03**	+14.30%	74.70	**77.77**	+4.11%	47.88	**61.62**	+28.70%
		FPR95 ↓	38.67	**38.33**	-0.88%	96.67	**91.33**	-5.52%	44.70	**42.00**	-6.04%	98.00	**94.00**	-4.08%
BZR	COX2	AUC ↑	75.00	**97.31**	+29.75%	34.69	**65.00**	+87.37%	80.00	**95.25**	+19.06%	41.80	**65.62**	+56.99%
		AUPR ↑	62.41	**97.17**	+55.70%	39.07	**62.89**	+60.97%	67.10	**94.34**	+40.60%	56.70	**67.22**	+18.55%
		FPR95 ↓	47.50	**15.00**	-68.42%	92.50	**80.00**	-13.51%	37.50	**12.50**	-66.67%	**97.50**	**97.50**	0.00%
TOX21	SIDER	AUC ↑	68.04	**71.27**	+4.75%	53.44	**58.25**	+9.00%	53.46	**69.39**	+29.80%	53.64	**55.67**	+3.78%
		AUPR ↑	69.28	**73.52**	+6.12%	56.81	**59.58**	+4.88%	56.02	**71.01**	+26.76%	**56.02**	**56.02**	0.00%
		FPR95 ↓	90.42	**89.53**	-0.98%	94.25	**92.72**	-1.62%	95.66	**90.55**	-5.34%	95.66	**89.66**	-6.27%
BBBP	BACE	AUC ↑	77.07	**80.64**	+4.63%	46.74	**50.53**	+8.11%	75.48	**78.54**	+4.05%	43.96	**51.28**	+16.65%
		AUPR ↑	68.41	**72.60**	+6.12%	45.35	**46.49**	+2.51%	69.32	**74.06**	+6.84%	44.77	**48.32**	+7.93%
		FPR95 ↓	71.92	**60.59**	-15.75%	92.12	**86.70**	-5.88%	76.85	**69.46**	-9.62%	94.09	**92.61**	-1.57%

Experiments

Case study: We visualize the learned graph prompts (i.e., amplifiers) for interpretability analysis.



(a) ID (b) ID (c) ID (d) OOD (e) OOD



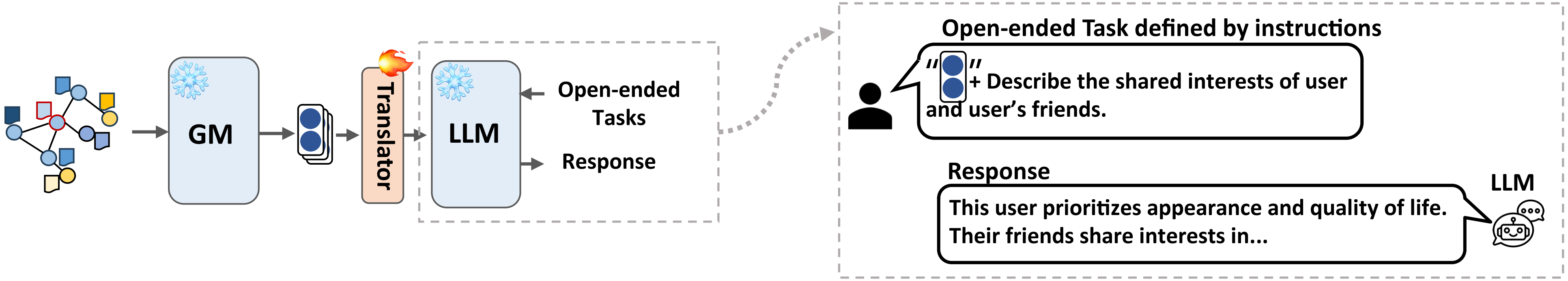
(a) ID (b) ID (c) ID (d) OOD (e) OOD

Motivation of GraphTranslator

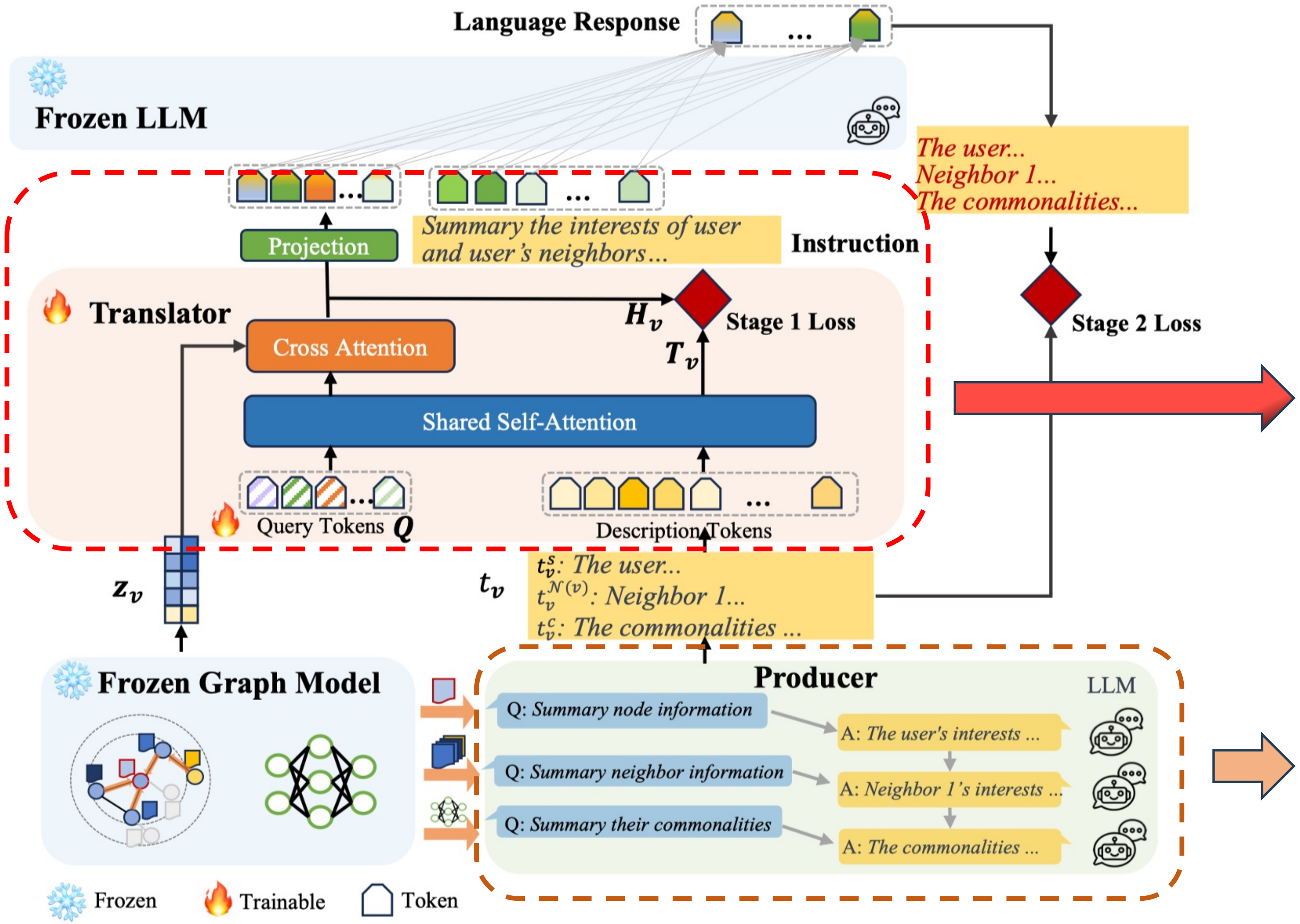
Motivation

- LLMs showcase impressive emergent abilities for open-ended tasks based on instructions, but struggle with processing complex graph data.
- Graph models (GMs) are often designed for encoding graph data into embeddings, while LLMs fail to directly process these embeddings.

Can we build a model that can bridge the gap between GM and LLM for open-ended tasks?



GraphTranslator



We propose a novel framework to align graph models (GMs) to LLM, named **GraphTranslator.**

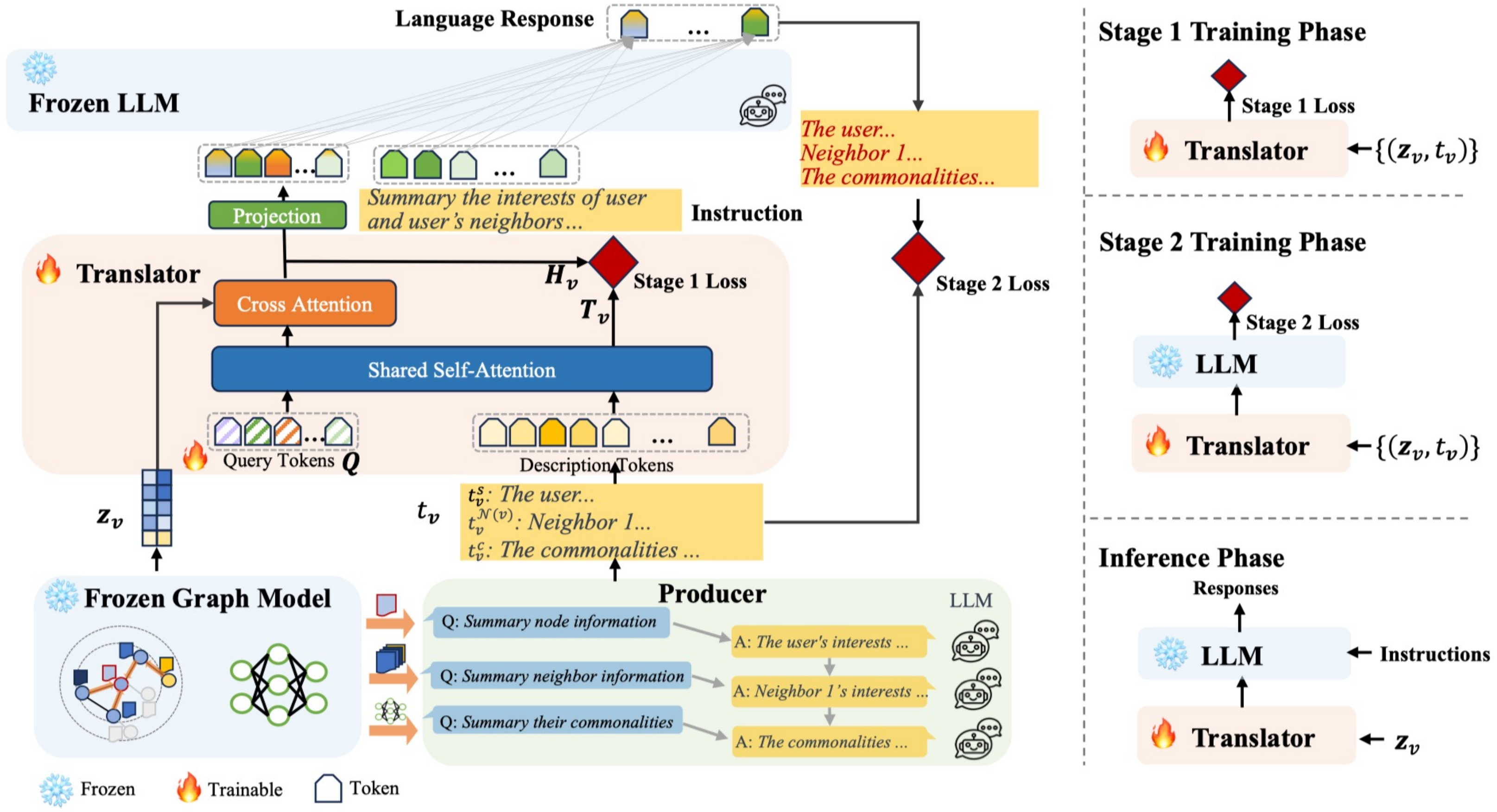
Translator

Translator aims to align GM and LLM by converting the learned node embedding into token representations.

Producer

We employ LLM to construct high-quality description text with Chain-of-Thought (COT).

GraphTranslator



- ☐ **Stage 1:** We obtain text embeddings with translator, then we train the translator through contrastive learning

- ☐ **Stage 2:** We use a linear layer to project the output of Translator module into the same dimension with the word embedding of LLM

Experiments

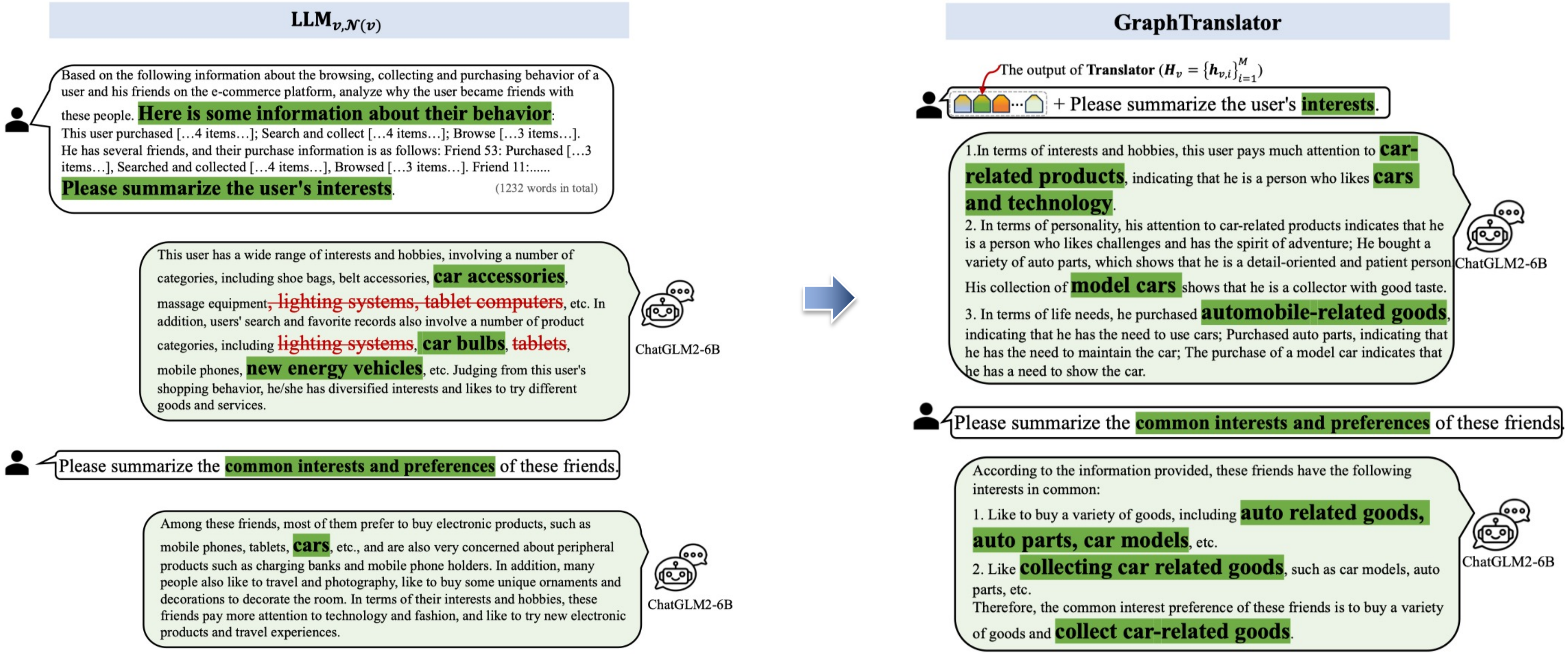
We conducted experiments on the Taobao and ArXiv datasets in zero-shot scenario.

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>

Experiments

We conducted QA experiment in Taobao dataset. GraphTranslator captures the preferences of users and their friends more accurate.



Outline

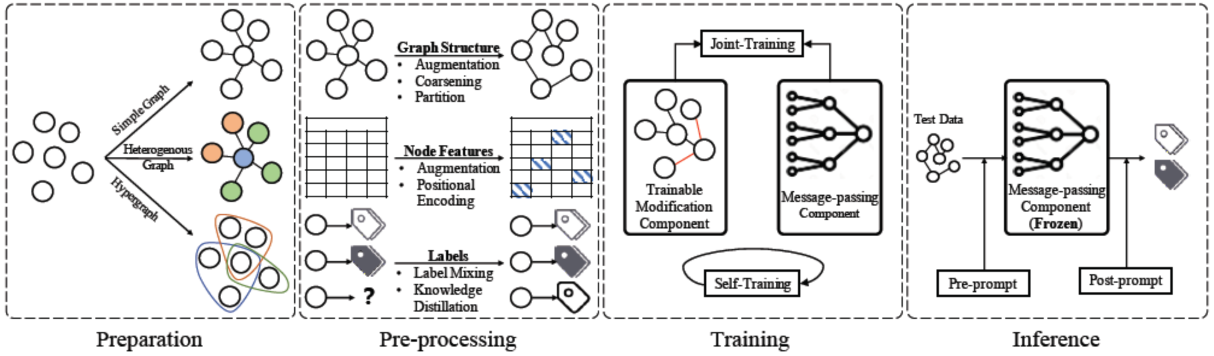
- Background
- Graph Foundation Model
- Our Recent Attempts
- Future Directions

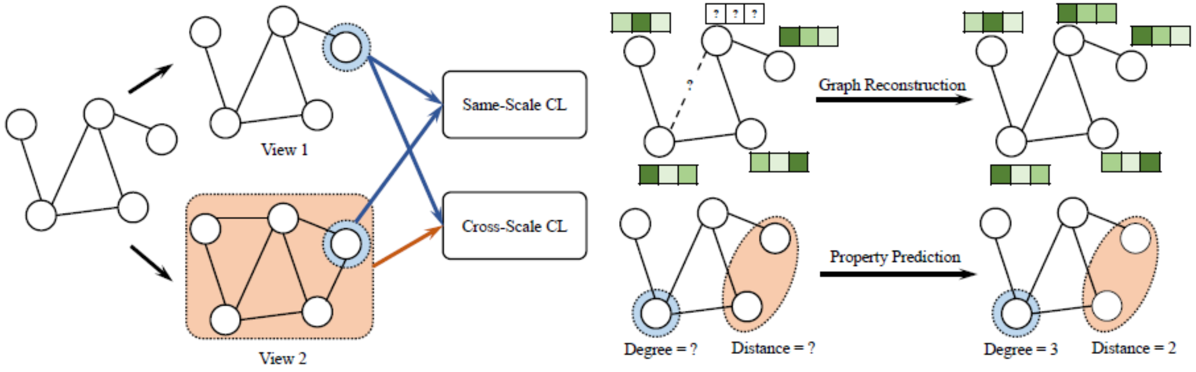
Future Directions

1. Data Quantity and Quality
    - Structure/Feature/Label Augmentation
    - Serialization for LLM-based Methods

2. Backbone and Learning Paradigm
    - Beyond the Transformer?
    - More Advanced Pretext Tasks

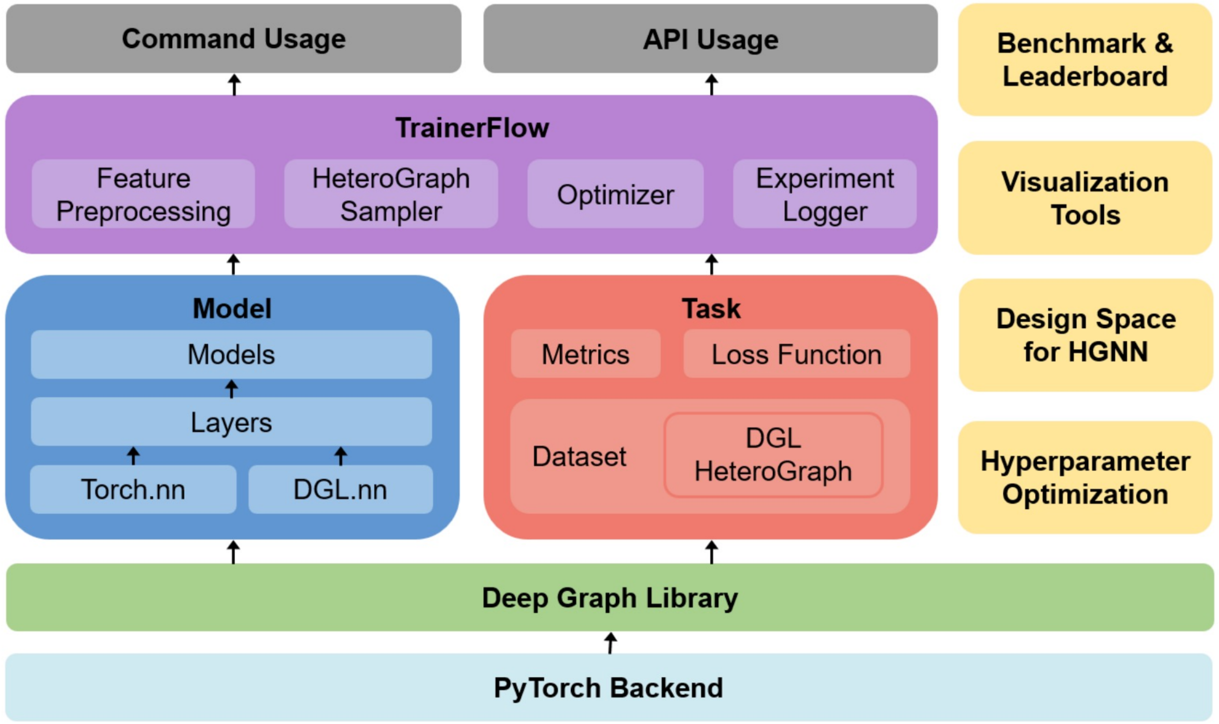
3. Application/Evaluation
    - Drug discovery, Urban Computing…
    - Human/AI Feedback
    - Safety/Privacy Issues



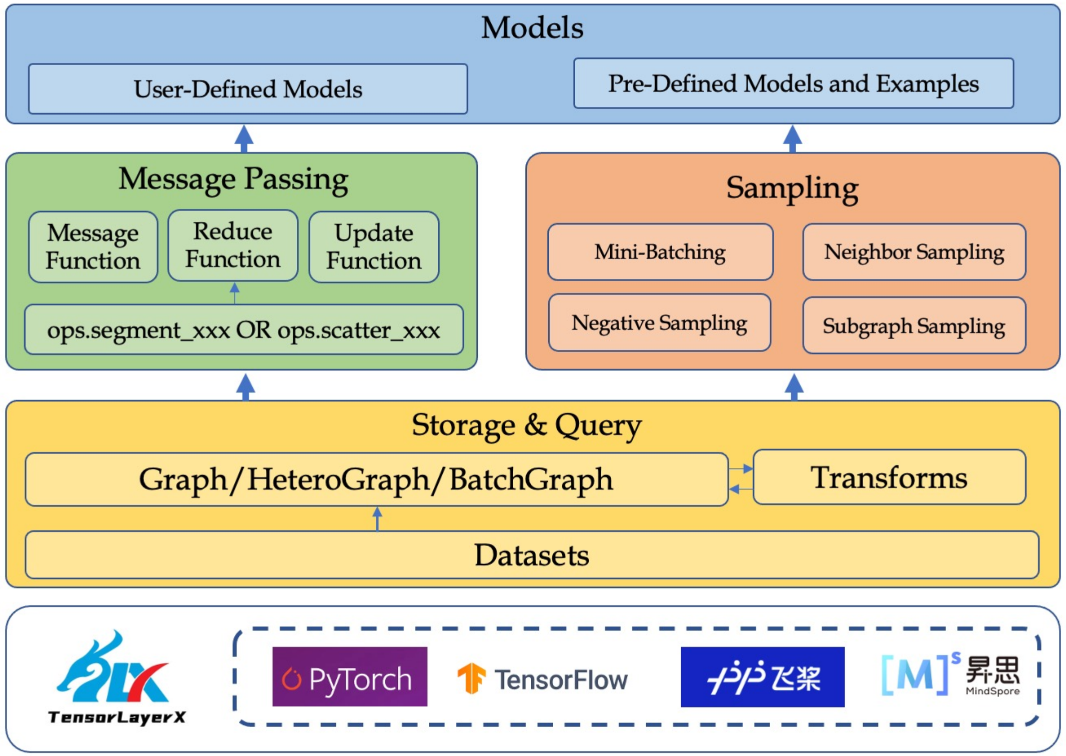


Open-source Graph Learning Platforms

OpenHGNN: The first heterogeneous graph neural network library



GammaGL: A GNN library supporting multiple deep learning backends



Yaoqi Liu, Cheng Yang, Tianyu Zhao, Hui Han, Siyuan Zhang, Jing Wu, Guangyu Zhou, Hai Huang, Hui Wang, Chuan Shi. GammaGL: A Multi-Backend Library for Graph Neural Networks. SIGIR 2023

Han H, Zhao T, Yang C, et al. OpenHGNN: An Open Source Toolkit for Heterogeneous Graph Neural Network. CIKM 2022

Thanks

Q&A