Towards Graph Foundation Models

WWW 2024 Tutorial

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Towards Graph Foundation Models
Part III: LLM & GNN+LLM Models

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Prepared by **Yuxia Wu**, Singapore Management University

Outline

- **LLM based Models**
  - Backbone Architecutures
  - Pre-training
  - Adaptation
- GNN+LLM based Models
  - Backbone Architecutures
  - Pre-training
  - Adaptation
- Summary and outlook

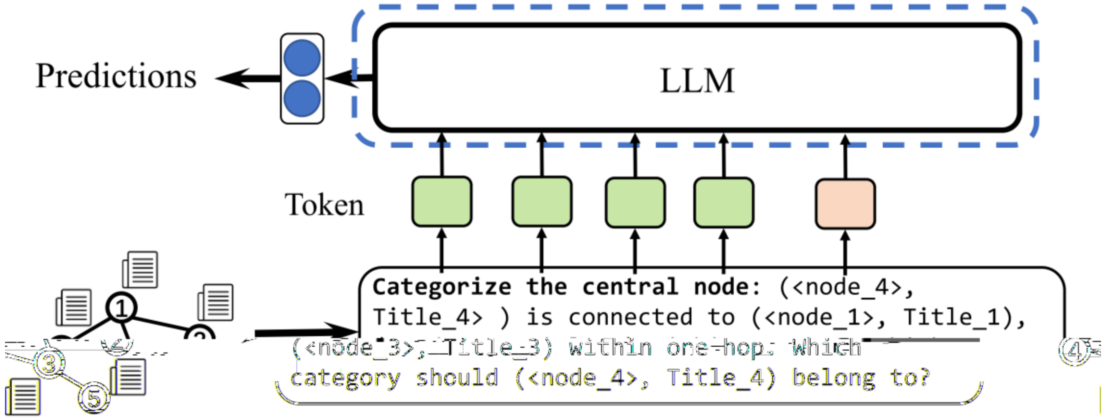
LLM-based Models

- ❑ **Backbone Architecutures**
- ❑ Pre-training
- ❑ Adaptation

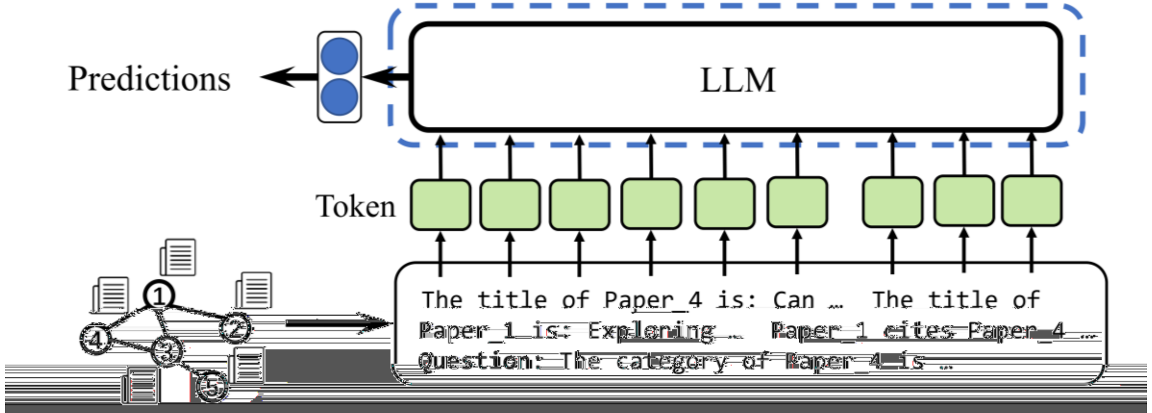
Model	Backbone Architecture			Pre-training	Adaptation
InstructGLM[157]	Graph-to-token	+	Flan-T5/LLaMA	MLM,LM	Manual Prompt Tuning
LLMtoGraph[71]	Graph-to-text	+	GPTs, Vicuna	LM	Manual Prompt Tuning
NLGraph[126]	Graph-to-text	+	GPTs	LM	Manual Prompt Tuning
GraphText[175]	Graph-to-text	+	GPTs	LM	Manual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

Backbone Architectures

- ❑ Graph-to-Token
  - ➢ Tokenize graph information to align it with LLM
- ❑ Graph-to-text
  - ➢ Describe graph information using natural language



(a) Graph-to-token.



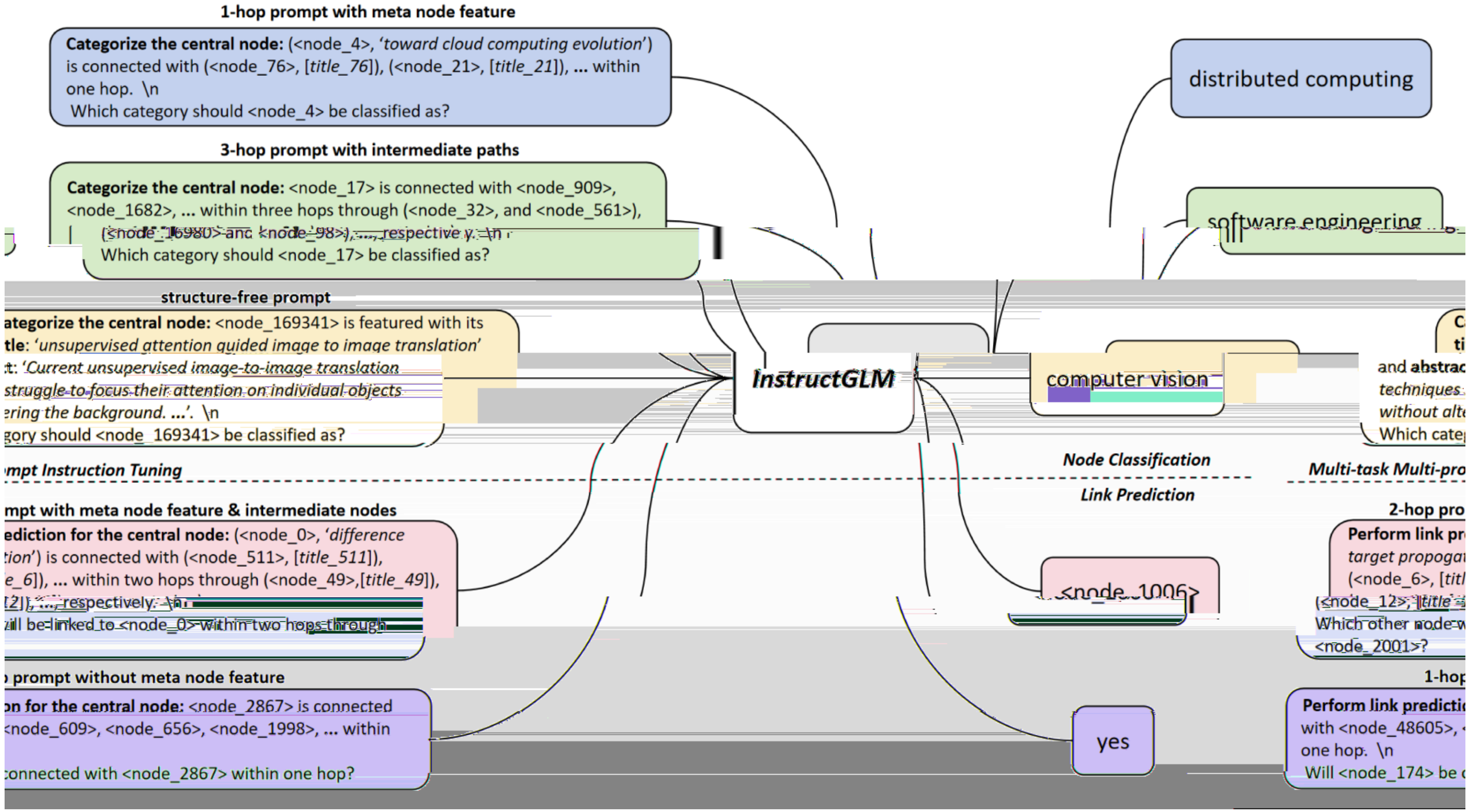
(b) Graph-to-text.

Graph-to-Token: GIMLET

- Integrating graph data with textual data
-

Graph-to-Token: InstructGLM

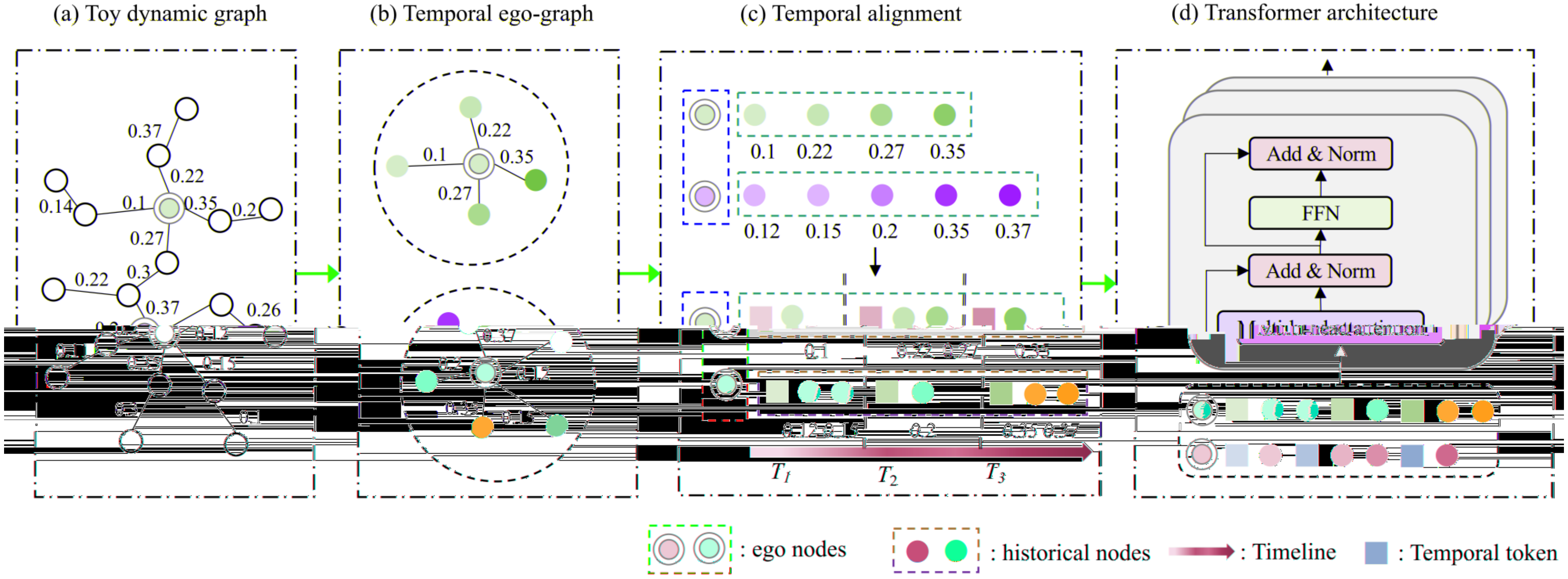
- Expand the vocabulary of the LLM by graph node features



Ye, et al. "Language is all a graph needs." *EACL 2024*.

Graph-to-Token: SimpleDyG

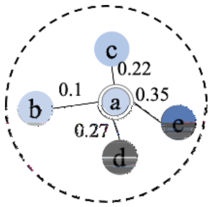
- Transformer-based approach for dynamic graphs
- Map a dynamic graph into a set of sequences



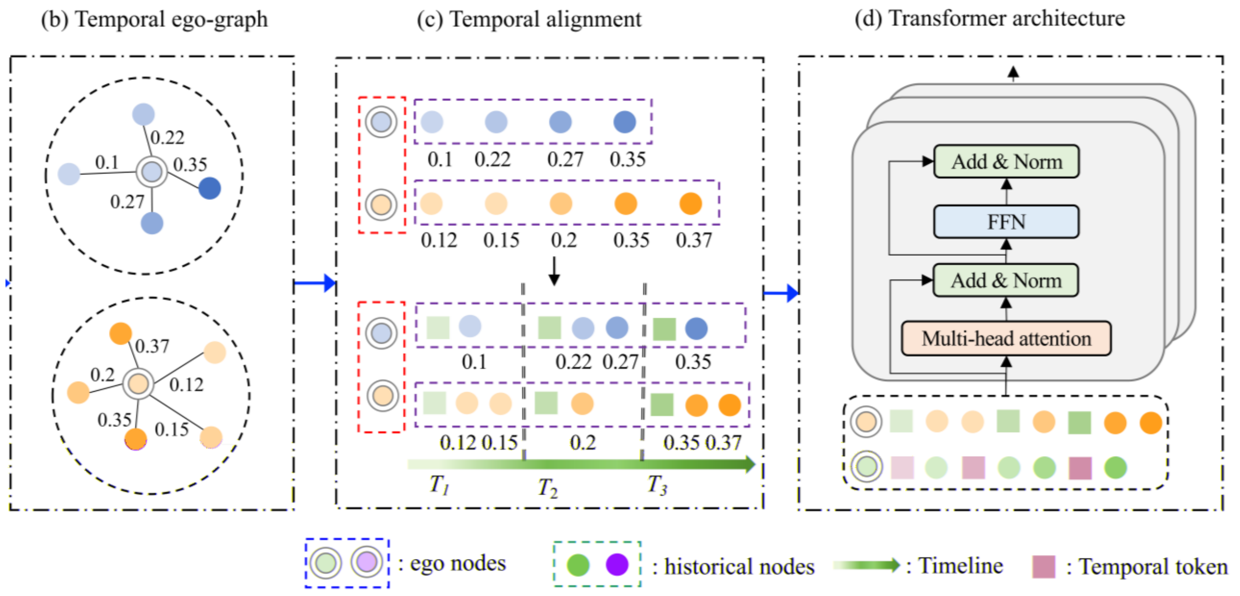
Wu, et al. "On the Feasibility of Simple Transformer for Dynamic Graph Modeling." *WWW’24*.

Graph-to-Token: SimpleDyG

- **Temporal ego-graph**



$$w_i = \langle b, c, d, e \rangle$$



- **Temporal alignment:**
  - Segment the time domain:

$$S_i^1 = \langle b \rangle \quad S_i^2 = \langle c, d \rangle \quad S_i^3 = \langle e \rangle$$

  - Sequence for Transformer:

$$x_i' = \langle |hist| \rangle, a, \langle |time1| \rangle, b, \langle |time2| \rangle, c, d, \langle |time3| \rangle, e, \langle |endofhist| \rangle$$

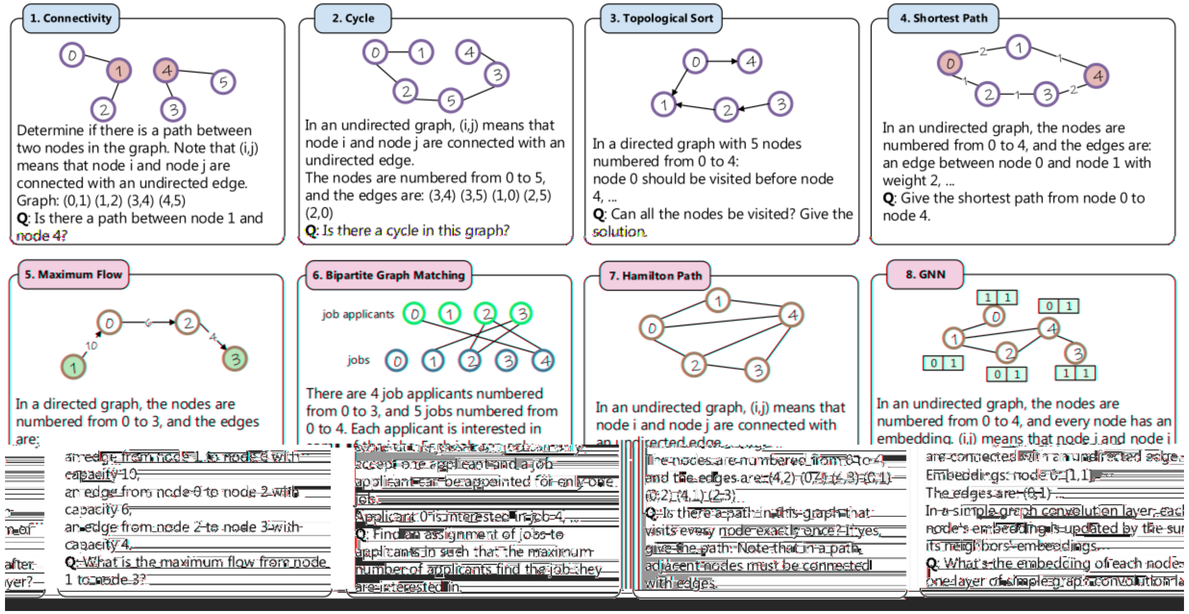
$$y_i' = \langle |pred| \rangle \langle |time4| \rangle S_i^4 \langle |endofpred| \rangle$$

Wu, et al. "On the Feasibility of Simple Transformer for Dynamic Graph Modeling." *WWW'24*.

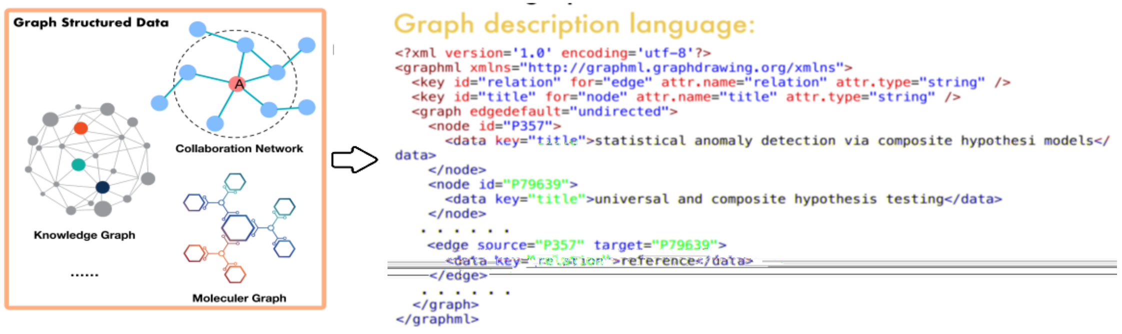
Graph-to-text

- ❑ Describe graph information for variours graphs and tasks

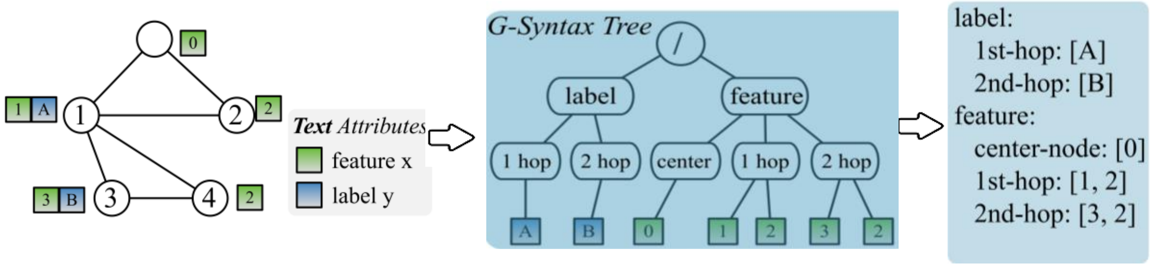
- ➢



- ➢Graph description language



- ➢Graph-Syntax Tree



Wang, et al. "Can language models solve graph problems in natural language?."
Guo, et al. "GPT4Graph: Can large language models understand graph structured data? an empirical evaluation and benchmarking."
Zhao, et al. "GraphText: Graph reasoning in text space."

LLM-based Models

- Backbone Architecutures
- **Pre-training**
- Adaptation

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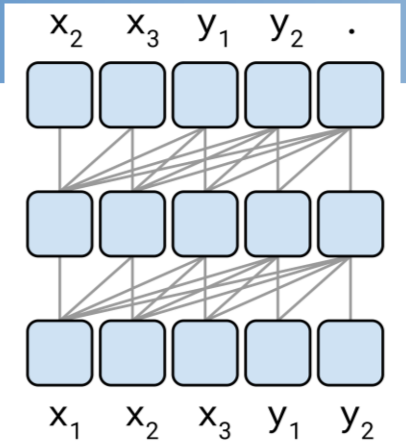
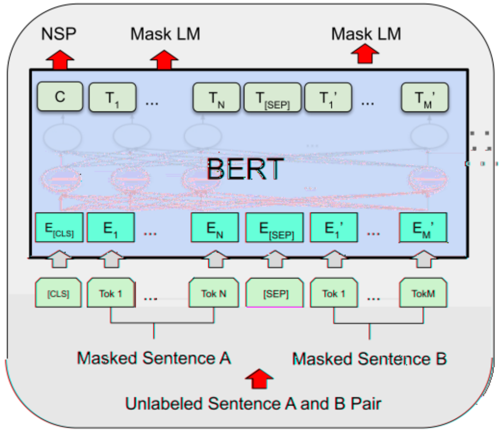
[illegible]	[illegible]	[illegible]	BERT, DeBERTa, Sentence-BERT, GPTs, LLaMA	[illegible]	[illegible]

Table 3. Details of approaches involved as LLM based models

Pre-training





Touvron, et al. "Llama: Open and efficient foundation language models." *CoRR'23*.
Ouyang, et al. "Training language models to follow instructions with human feedback." *NeurIPS'22*.
Devlin, et al. "BERT: Pre-training of deep bidirectional transformers for language understanding." *CoRR'18*.
Raffel, et al. "Exploring the limits of transfer learning with a unified text-to-text transformer." *JMLR'20*.

LLM-based Models

- ❑ Backbone Architecutures
- ❑ Pre-training
- ❑ **Adaptation**

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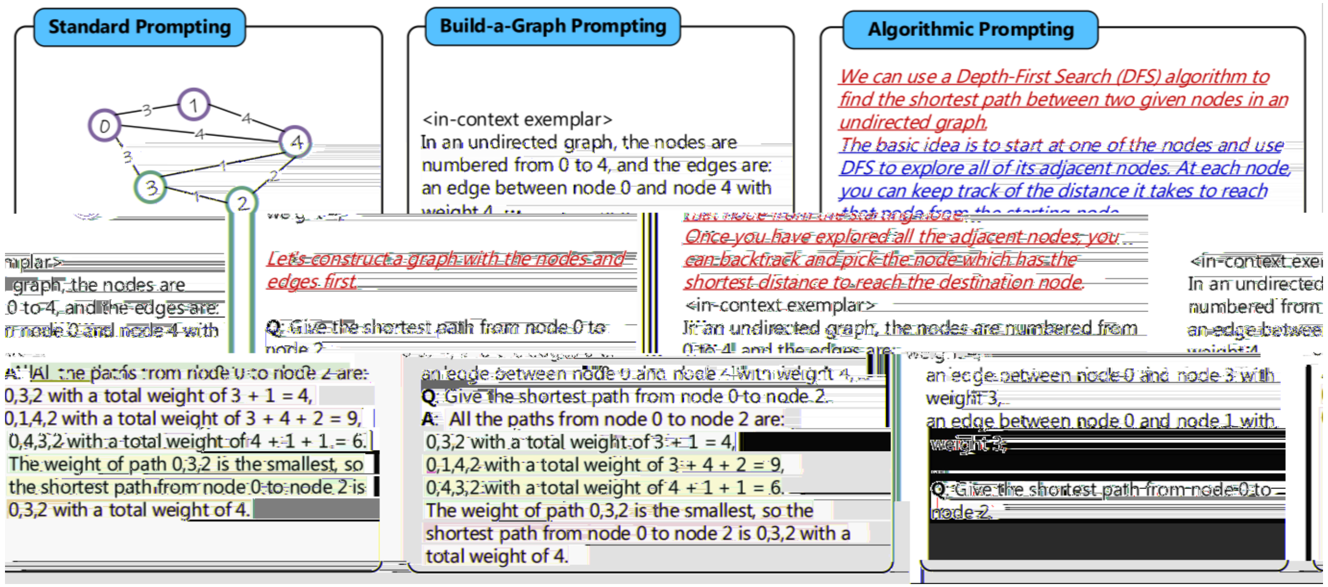
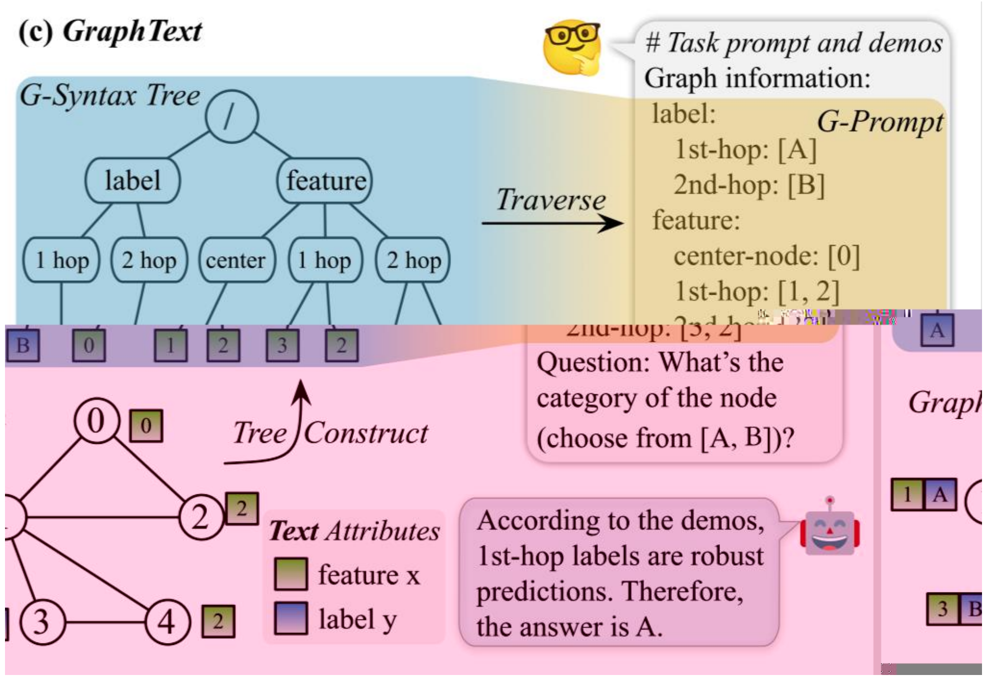
Graph-LLM[50]	Graph-to-text	+	BERT, DeBERTa, Sentence-BERT, GPTs, LLaMA	MLM,LM	Manual Prompt Tuning + Automatic Prompt Tuning

Table 3. Details of approaches involved as LLM based models

Adaptation

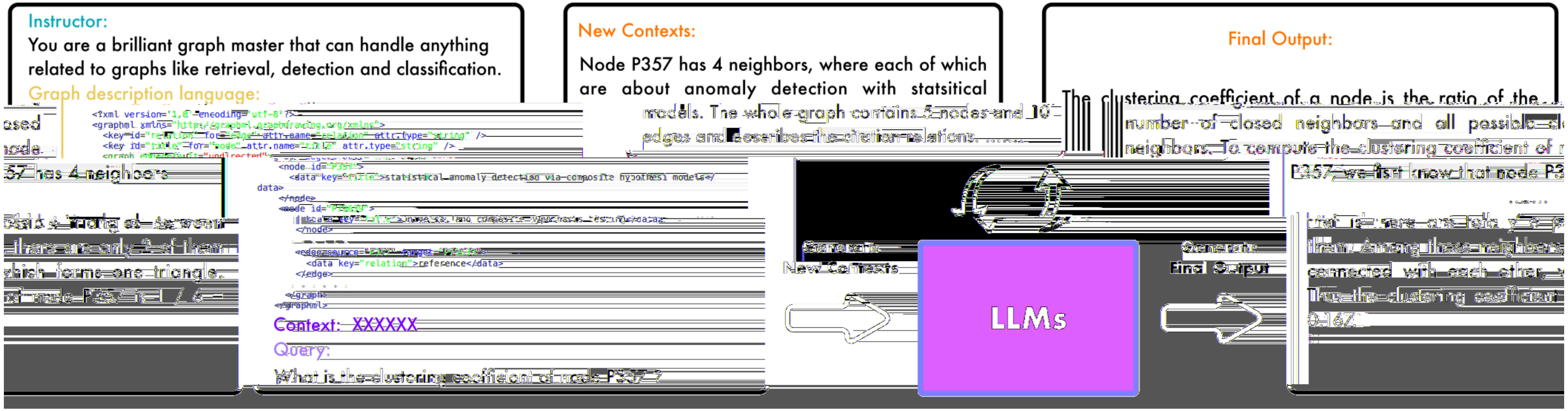




Wang, et al. "Can language models solve graph problems in natural language?." *NeurIPS*'23
Zhao, et al. "GraphText: Graph reasoning in text space."

Adaptation

- ❑ Manual Prompting: Graph information, task descriptions
- ❑ Automatic Prompting: LLMs → generate the context
  - ➢ Ask LLM generate graph/neighbor summarization



Guo, et al. "Gpt4graph: Can large language models understand graph structured data? an empirical evaluation and benchmarking."
Chen, et al. "Exploring the potential of large language models (llms) in learning on graphs." *ACM SIGKDD Explorations Newsletter 2024*

Outline

- GNN+LLM based Models

GNN+LLM based Models

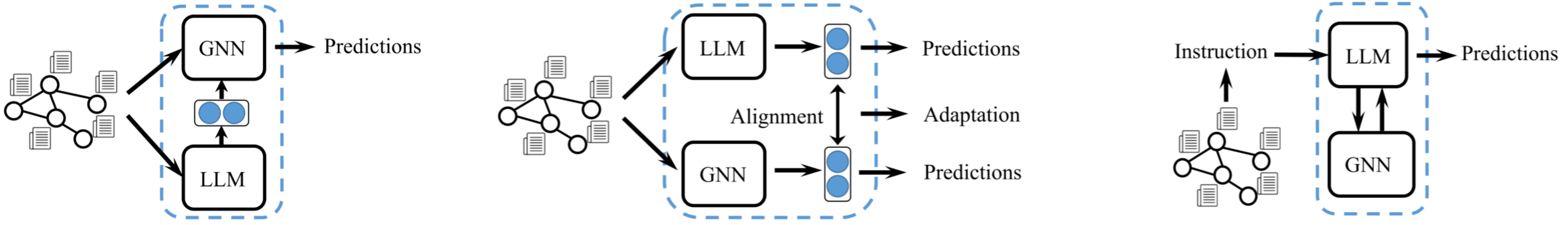
- ❑ **Backbone Architecutures**
- ❑ Pre-training
- ❑ Adaptation

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
GALM [147]	GNN-centric	Graph Reconstruction	Vanilla 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

Table 4. Details of approaches involved as GNN+LLM based models

Backbone Architectures

- GNN-centric Methods
  - LLMs extract node features from raw data; GNNs make predictions
- Symmetric Methods
  - Align the embeddings of GNN and LLM
- LLM-centric Methods
  - Utilize GNNs to enhance the performance of LLM

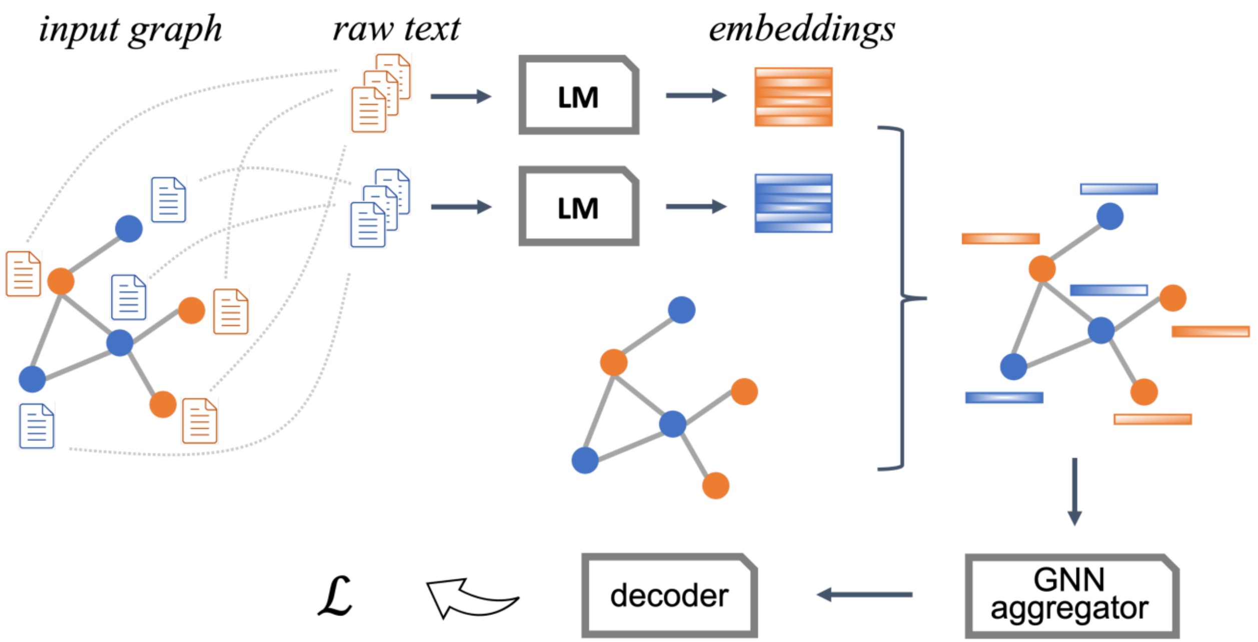


(a) GNN-centric methods. (b) Symmetric methods. (c) LLM-centric methods.

GNN-centric Methods: GaLM

❑ The backbone model:

Raw text → LMs → GNN aggregator → decoder



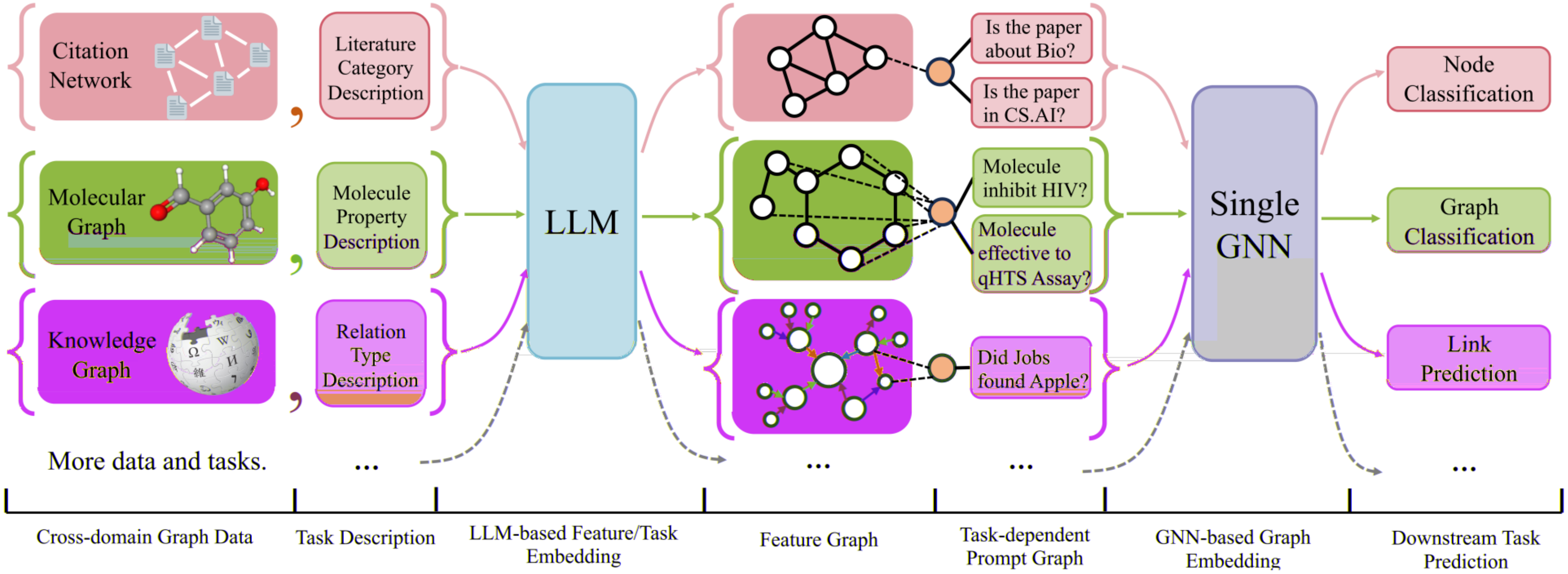
Xie, et al. "Graph-aware language model pre-training on a large graph corpus can help multiple graph applications." .

GNN-centric Methods: One for all

- The backbone model:

Text-attributed graph
Task description

LLMs → Prompted graph → GNN → Downstream tasks

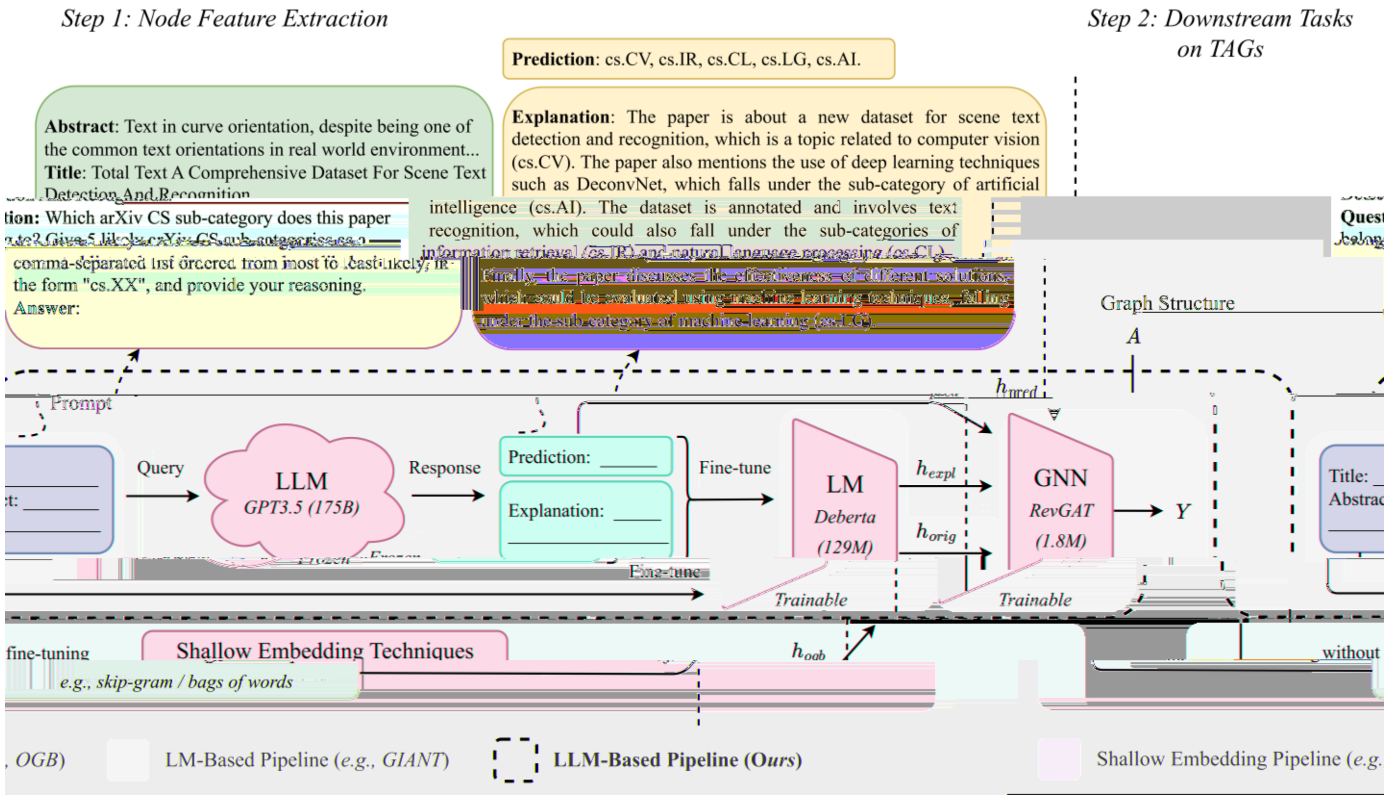


Liu, et al. "One for all: Towards training one graph model for all classification tasks."

GNN-centric Methods: TAPE

❑ The backbone model:

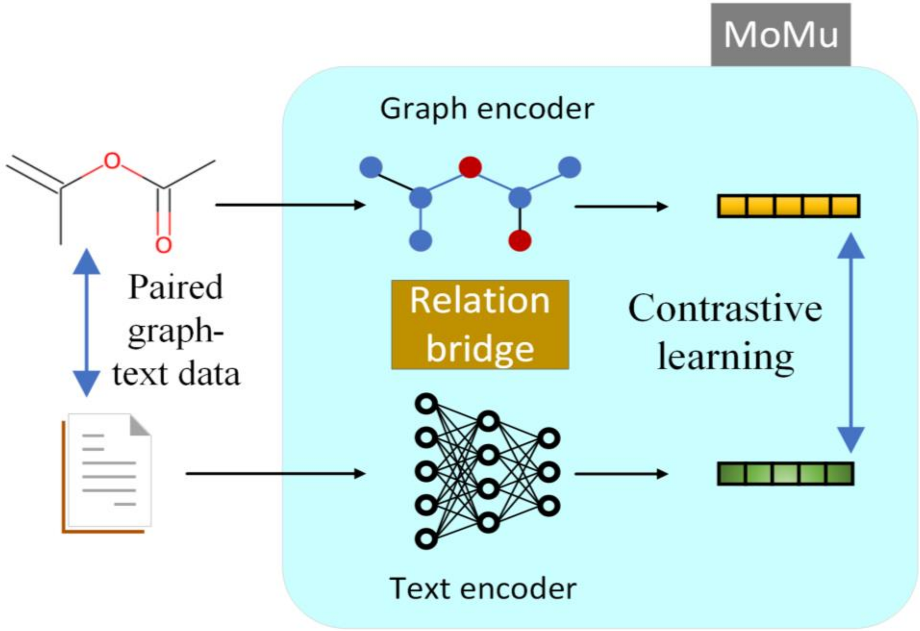
Textual attributes → LLM → Prediction & Explanation → Fine-tune LM → Node features → GNN

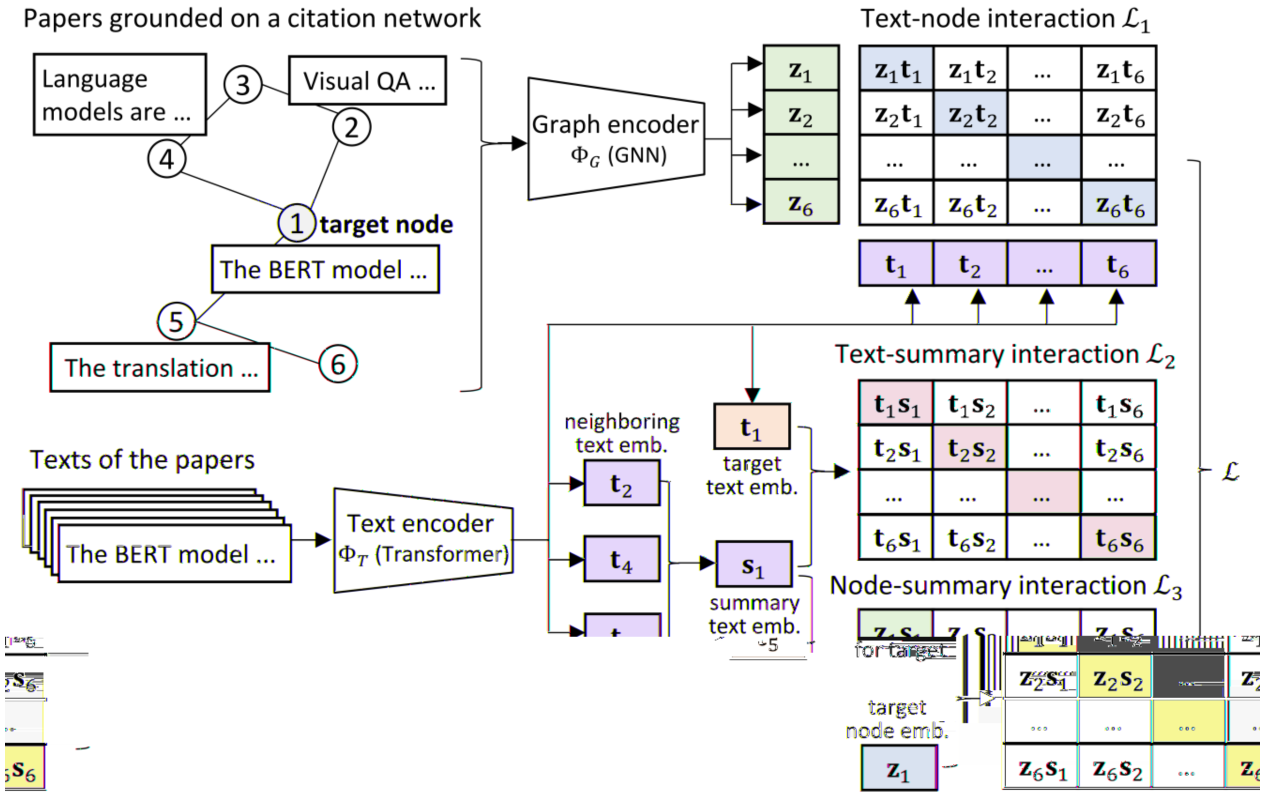


He, et al. "Harnessing explanations: LLM-to-LM interpreter for enhanced text-attributed graph representation learning."

Symmetric Methods: MoMu, G2P2

- The backbone model:
  - Dual encoders: Graph & Text encoder
  - Contrastive Learning





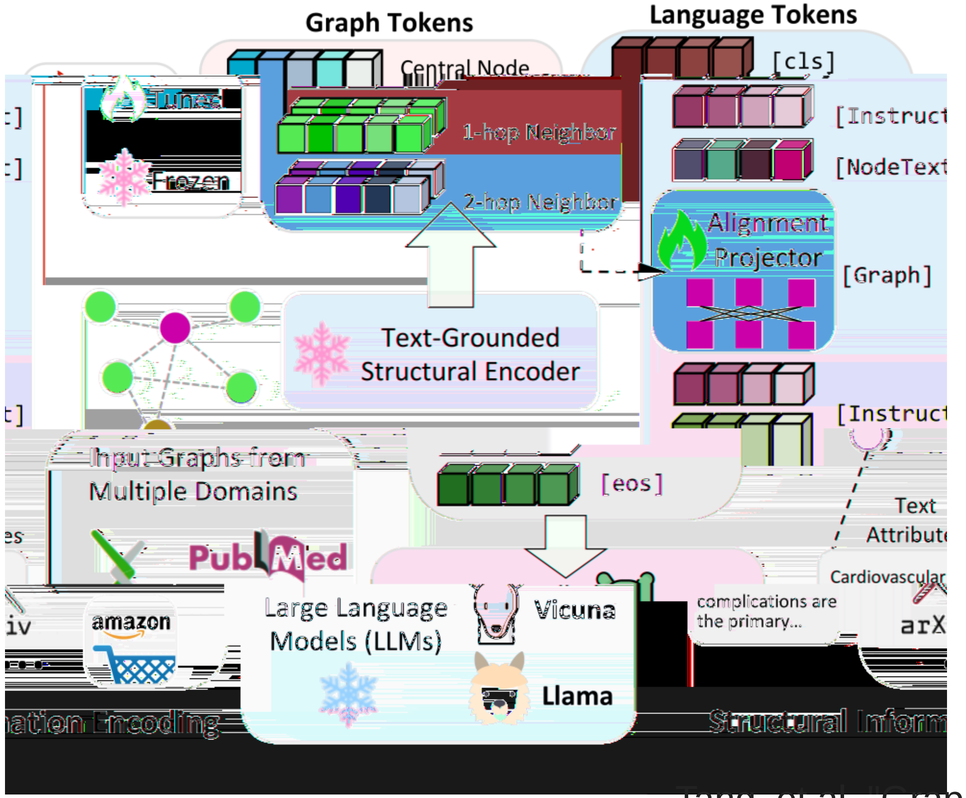
Su, et al. "A molecular multimodal foundation model associating molecule graphs with natural language." .

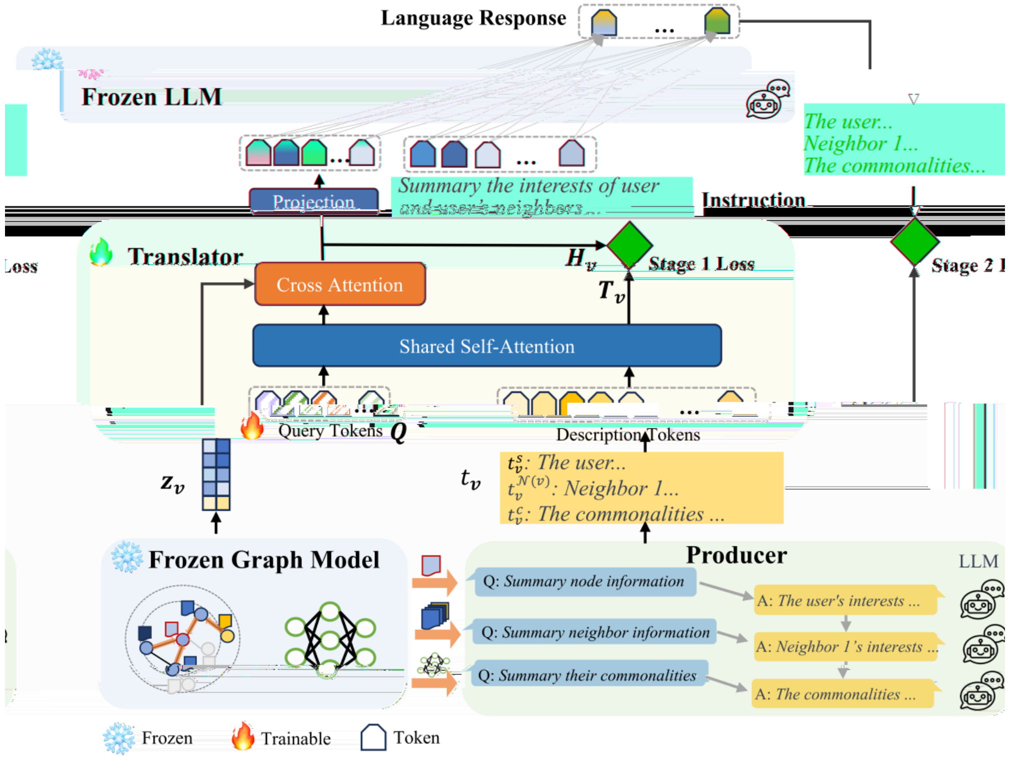
Wen, et al. "Augmenting low-resource text classification with graph-grounded pre-training and prompting." .

LLM-centric Methods: GraphGPT, GraphTranslator

- ❑ The backbone model:

  Graph → GNN → Projection → LLM





Tang, et al. "GraphGPT: Graph instruction tuning for large language models."

Zhang, et al. "GraphTranslator: Aligning Graph Model to Large Language Model for Open-ended Tasks."

GNN+LLM based Models

- ❑ Backbone Architecutures
- ❑ **Pre-training**
- ❑ Adaptation

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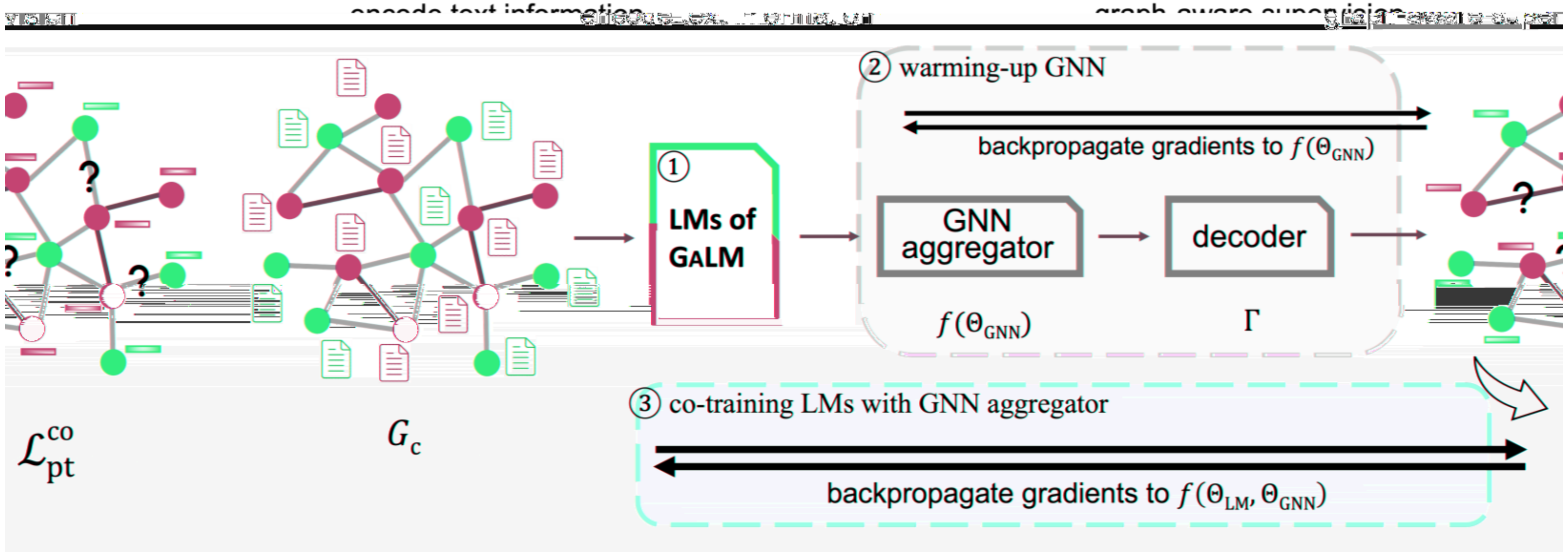
Table 4. Details of approaches involved as GNN+LLM based models

Pre-training

- GNN or LLM-based
  - Masked Language Modeling
  - Language Modeling
  - Text-Text Contrastive Learning
  - Graph reconstruction
- Alignment-based
  - Graph-Text Contrastive Learning

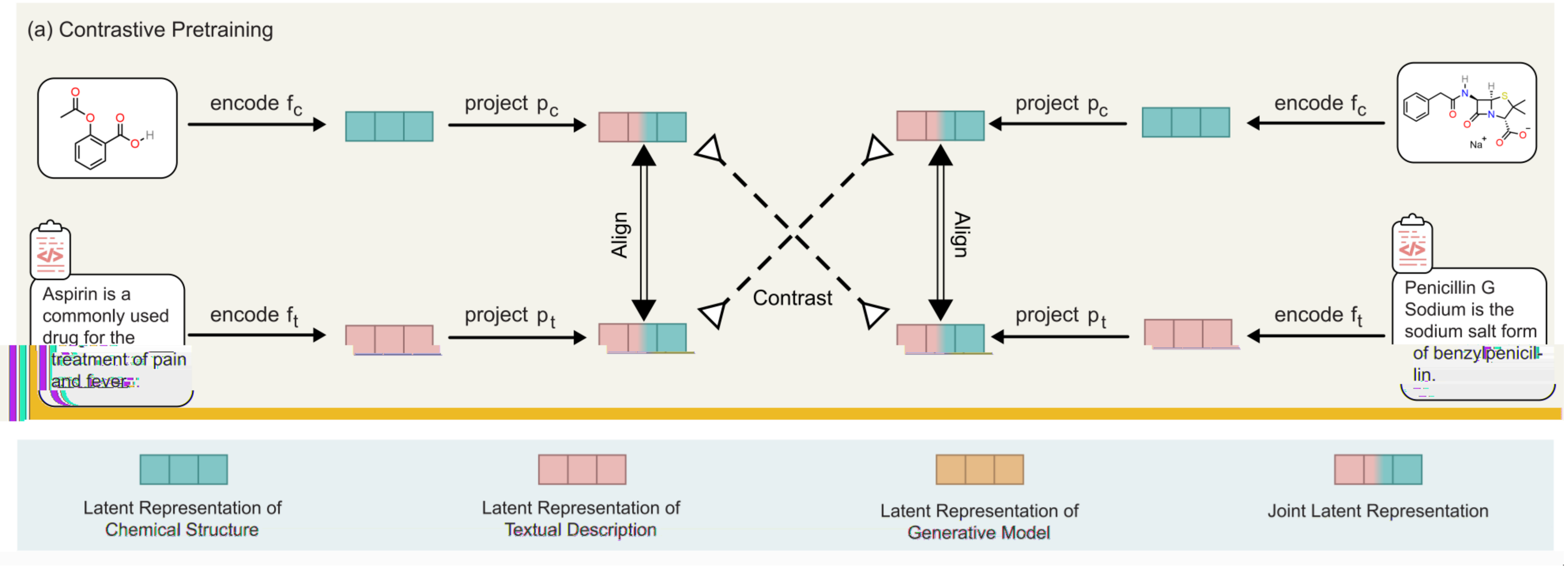
GNN or LLM-based: GaLM



Xie, et al. "Graph-aware language model pre-training on a large graph corpus can help multiple graph applications." .

Alignment-based: MoleculeSTM

- ❑Graph-Text Contrastive Learning (GTCL)
  - ➢ Map the graph and text representations extracted to a joint space using two projectors (p_c and p_t) via contrastive learning



Liu, et al. "Multi-modal molecule structure–text model for text-based retrieval and editing." *Nature Machine Intelligence* 2023

Alignment-based: G2P2

- $s_i = \frac{1}{\cdots} \sum_{j \in \mathcal{N}_i} t_j$

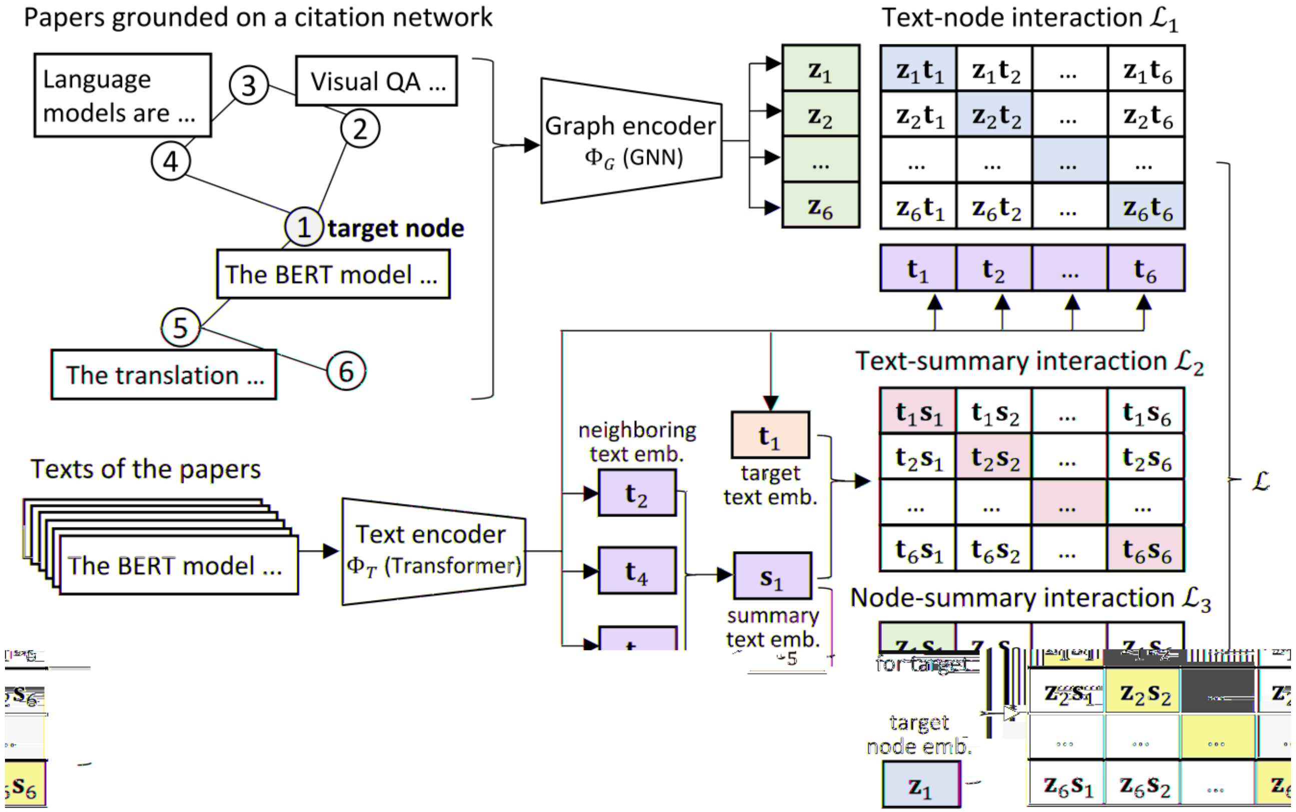


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Table 4. Details of approaches involved as GNN+LLM based models

Adaptation

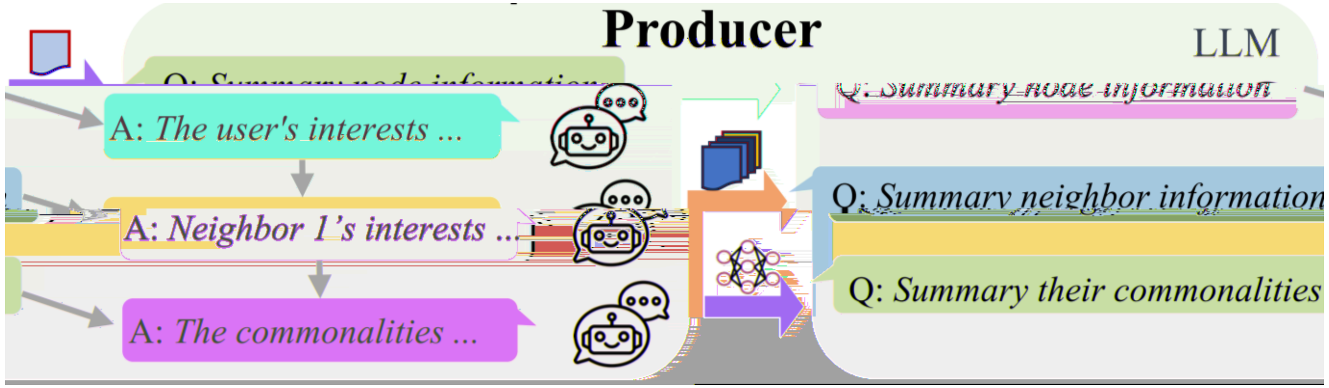
PEFT: GraphTranslator

- Frozen:
  - Graph Model
  - Large Language Model
- Tunable:
  - Producer Module
    - Construct alignment data
  - Translator Module
    - Convert node representations into tokens for LLM prediction

Zhang, et al. "GraphTranslator: Aligning Graph Model to Large Language Model for Open-ended Tasks."

PEFT: GraphTranslator

- Producer:
  - CoT) ->LLM->high-quality description
    - node information
    - neighbor information
    - commonalities



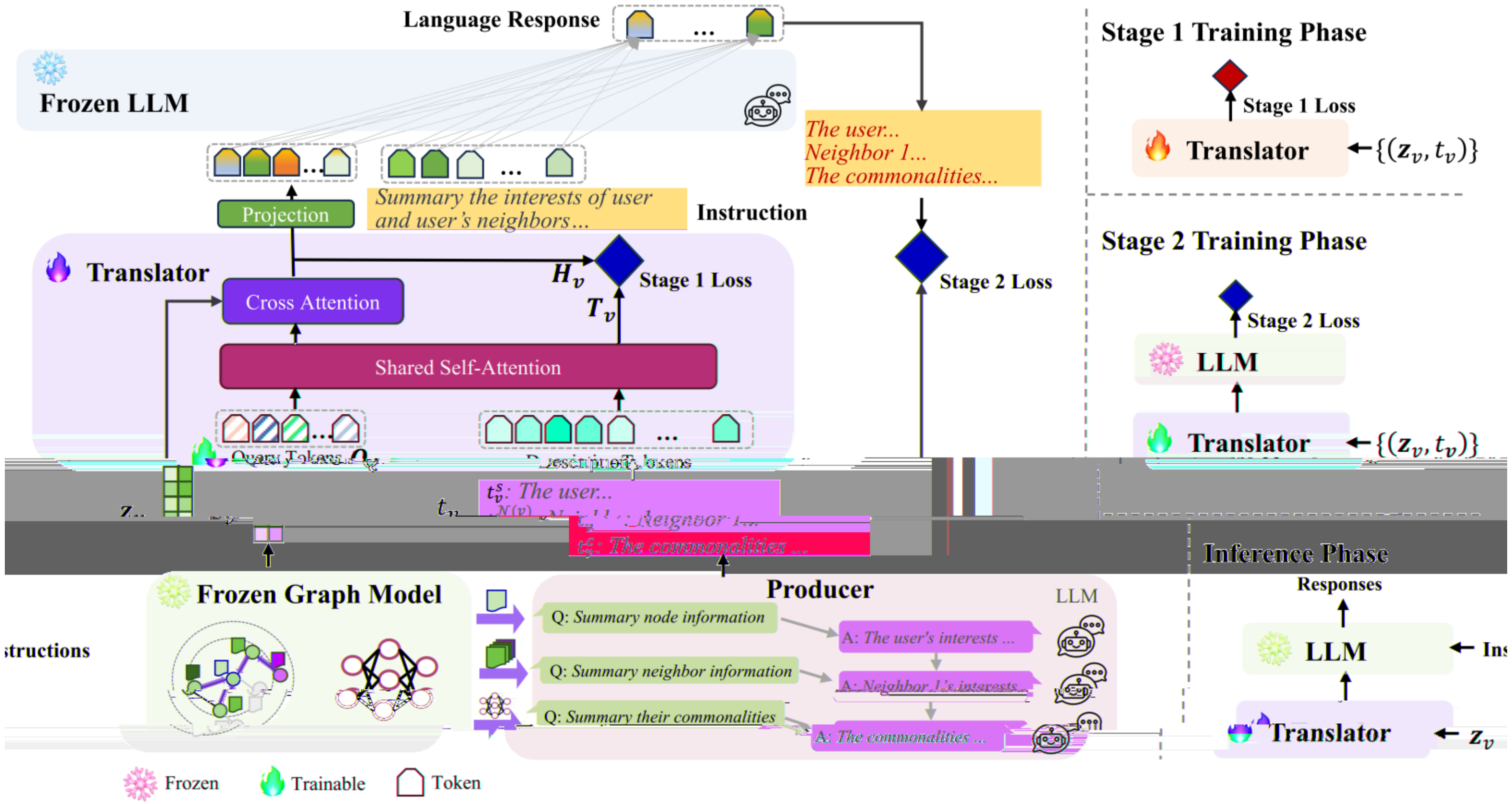
- Prompt template:

Dataset	Step	Prompt
Taobao	User behavior summary	User Behavior Description: <User Behavior Description>. Please summarize the characteristics of this user according to the product behavior information. The answer format is: What kind of characteristics does the user have in terms of interests, hobbies, personality traits, and life needs
	Neighbor behavior summary	Neighbor Behavior Description: <Neighbor Behavior Description>. Please summarize most of the similarities that this user's friends have based on the product behavior information. The answer format is: What do several friends of this user have in common in interests, hobbies, personality traits, and life needs?

Zhang, et al. "GraphTranslator: Aligning Graph Model to Large Language Model for Open-ended Tasks."

PEFT: GraphTranslator

- Training: Only fine-tune Translator and Projection

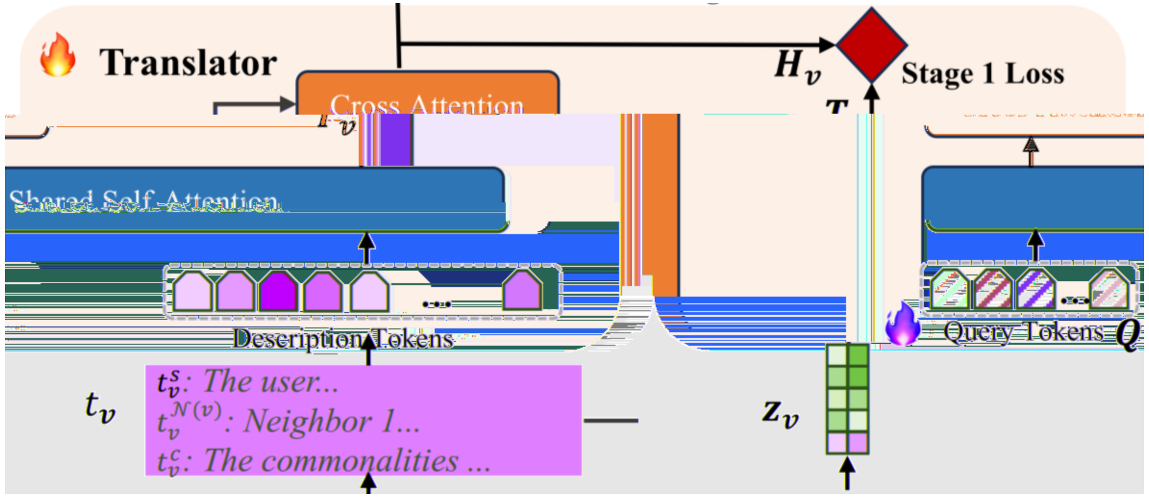


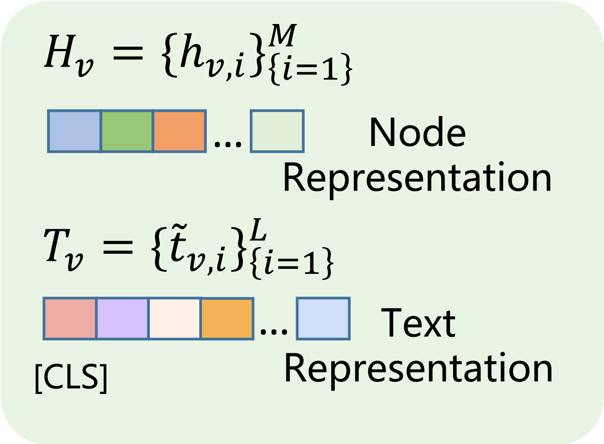
- Stage1: Align graph-text
- Stage2: Align graph-LLM

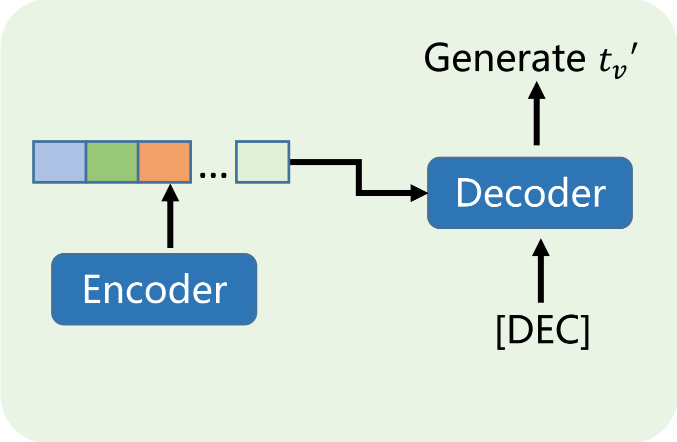
Zhang, et al. "GraphTranslator: Aligning Graph Model to Large Language Model for Open-ended Tasks."

PEFT: GraphTranslator

❑ Training: Stage 1







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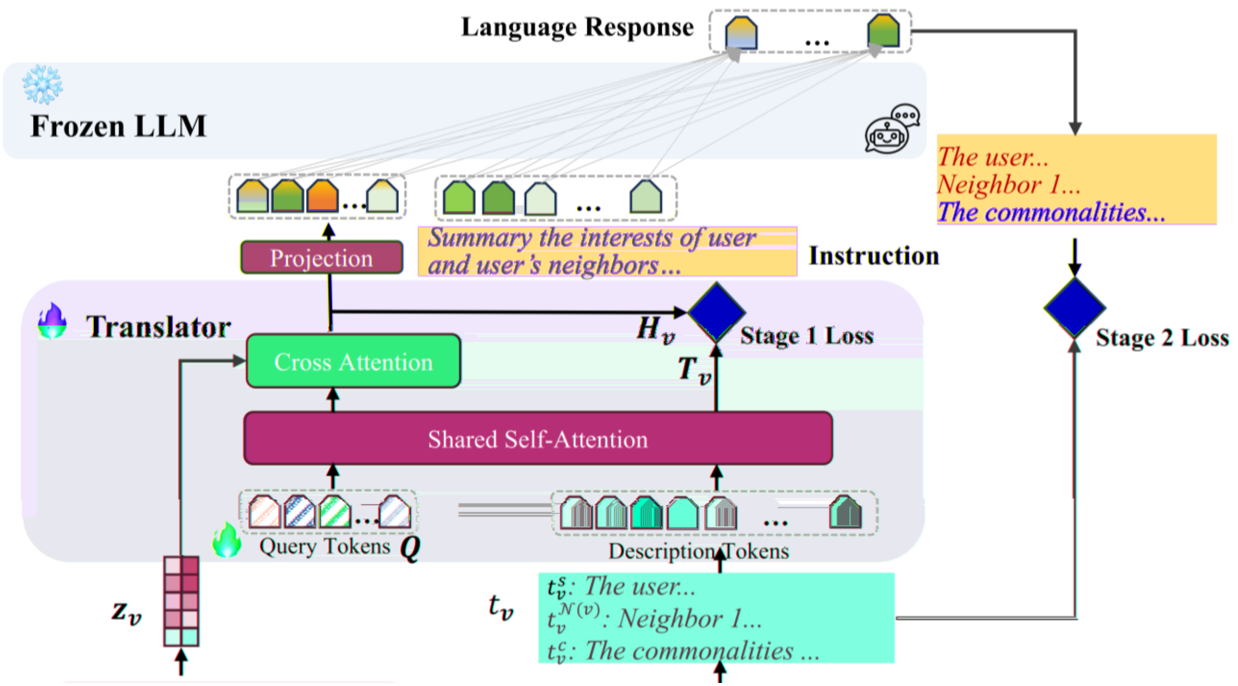
PEFT: GraphTranslator

❑ Training: Stage 2

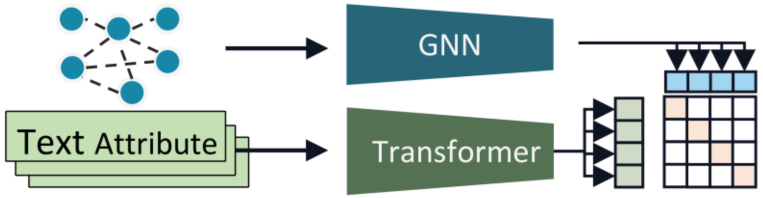


- Projection:
  - A linear layer: project H_v to token representation space of LLM
- Concatenate:
  - Connect the projected representation with the human instruction and feed into LLM
- Fine-tune Translator
  - Alignn the response text of LLM with the actual descriptive text

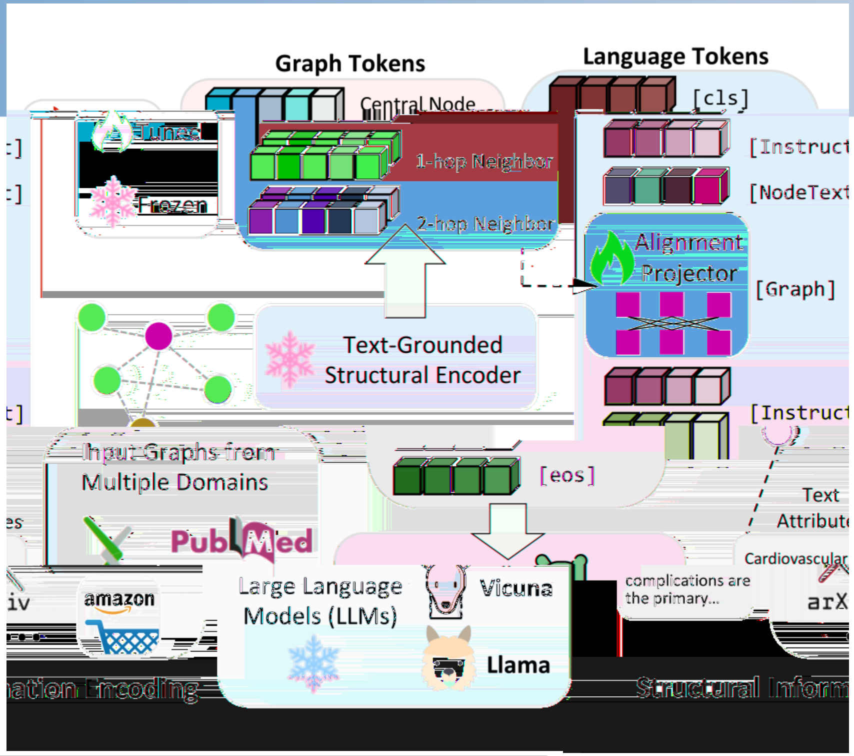
Zhang, et al. "GraphTranslator: Aligning Graph Model to Large Language Model for Open-ended Tasks." WWW'24

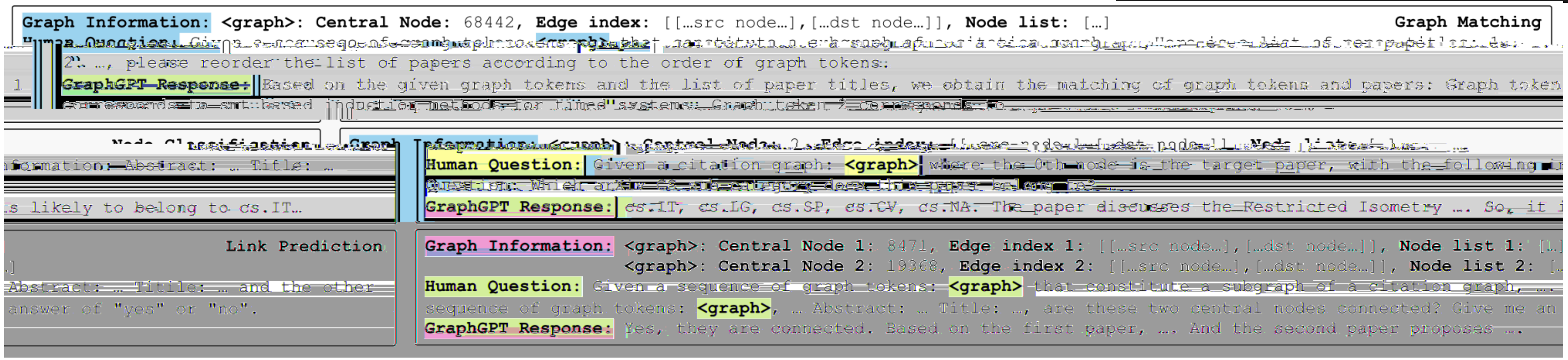
PEFT: GraphGPT

- ❑ Graph: Text-Grounded Structural Encoder



- ❑ Projector: Map graph representation to LLM
- ❑ Instruction Tuning: Only fine-tune projector

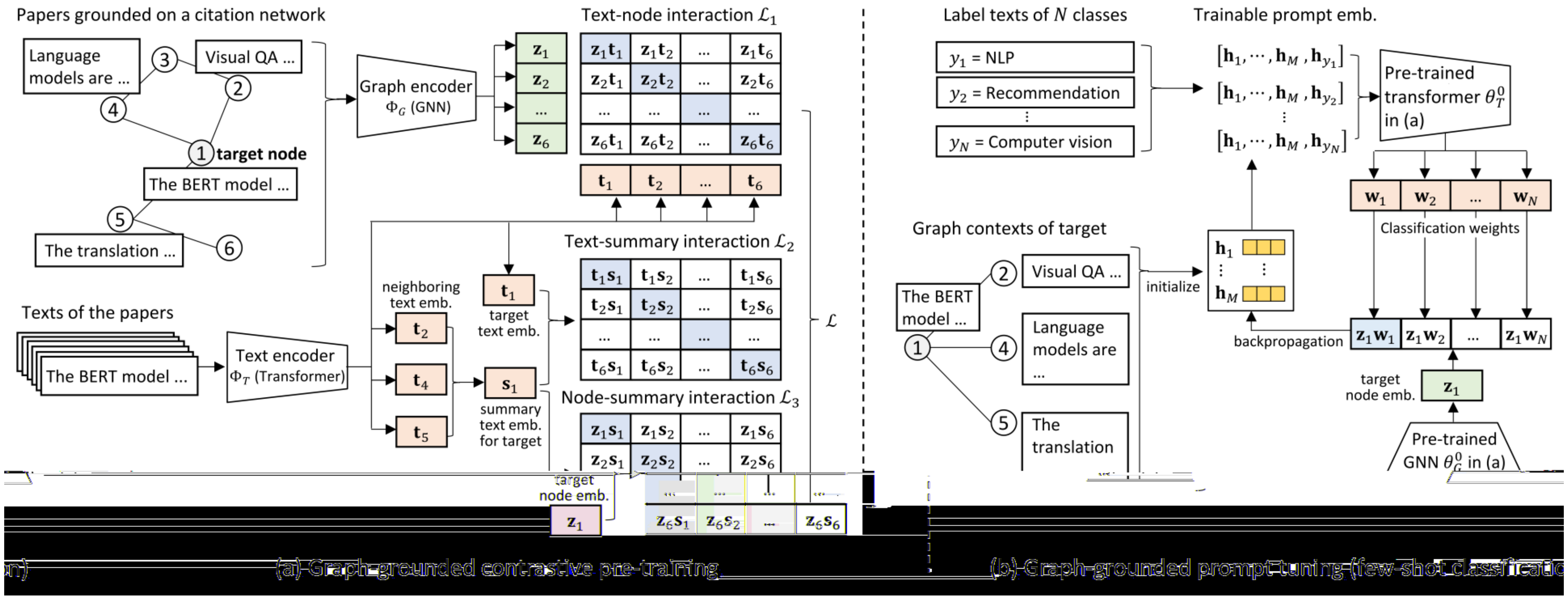




Tang, et al. "GraphGPT: Graph instruction tuning for large language models."

Prompt-Tuning: G2P2

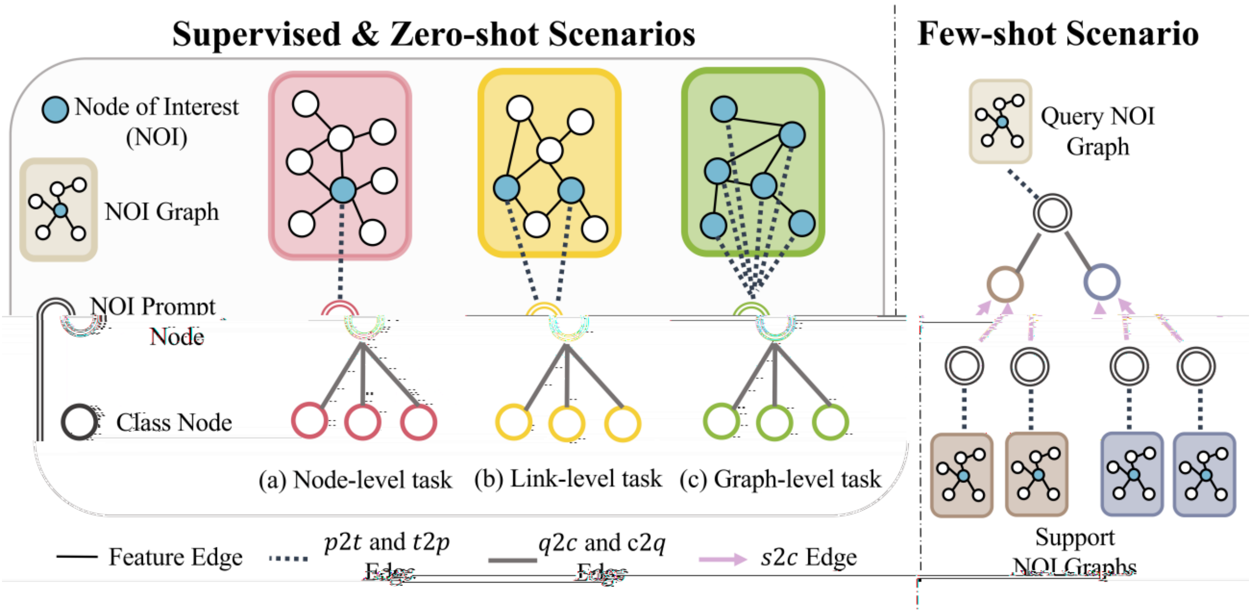
- Learnable prompts: $[h_1, \cdots h_M, h_{CLASS}]$
- Tuning prompts with limited labeled data for efficient adaptation



Wen, et al. "Augmenting low-resource text classification with graph-grounded pre-training and prompting." .

Prompt-Tuning: One for all

- ❑ NOI (Node of Interest):
  - ➢ Node-level: node
  - ➢ Link-level: node pair
  - ➢ Graph-level: subgraph



- ❑ NOI Prompt Node

> **Text feature of the NOI prompt node:** Prompt node. <*task description*>.
> **Example:** Prompt node. Graph classification on molecule properties.
> **Example:** Prompt node. Node classification on the literature category of the paper.

- ❑ Class Node

> **Text feature of class node:** Prompt node. <*class description*>.
> **Example:** Prompt node. Molecule property. The molecule is effective in: ...
> **Example:** Prompt node. Literature Category. cs.AI (Artificial Intelligence). Covers all areas of AI except Vision ...

Liu, et al. "One for all: Towards training one graph model for all classification tasks."

Outline

- LLM based Models
  - Backbone Architecutures
  - Pre-training
  - Adaptation
- GNN+LLM based Models
  - Backbone Architecutures
  - Pre-training
  - Adaptation
- **Summary and outlook**

Summary and outlook

❑ Summary

- ➢ Leveraging LLMs facilitates a unified approach to various graph tasks by describing them in natural language.
- ➢ Merging graph data, text, and other modalities into LLMs creates a promising path for graph foundation models.
- ➢ Combining GNNs and LLMs leads to improved performance in graph-related tasks.

Summary and outlook

- Outlook
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