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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Outline

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

LLM-based Models

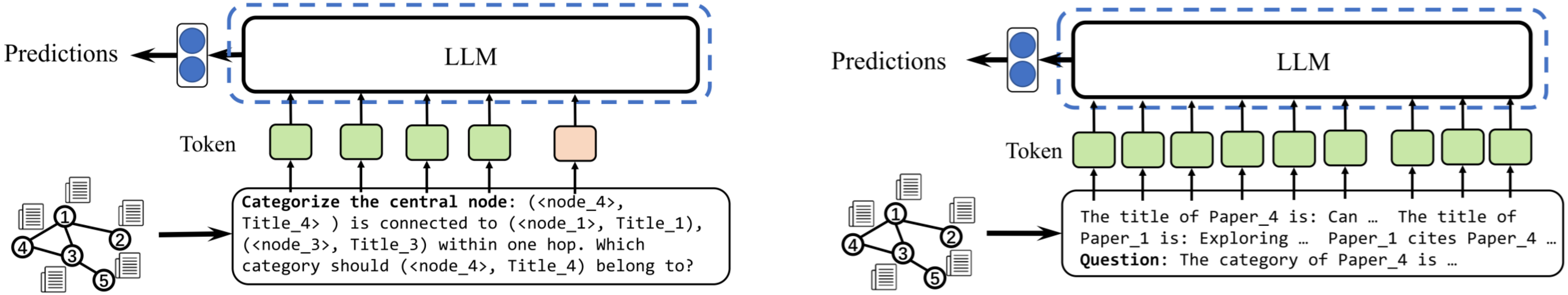
- ❑ **Backbone Architecutures**
- ❑ Pre-training
- ❑ Adaptation

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
Graph-LLM[9]	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

Backbone Architectures

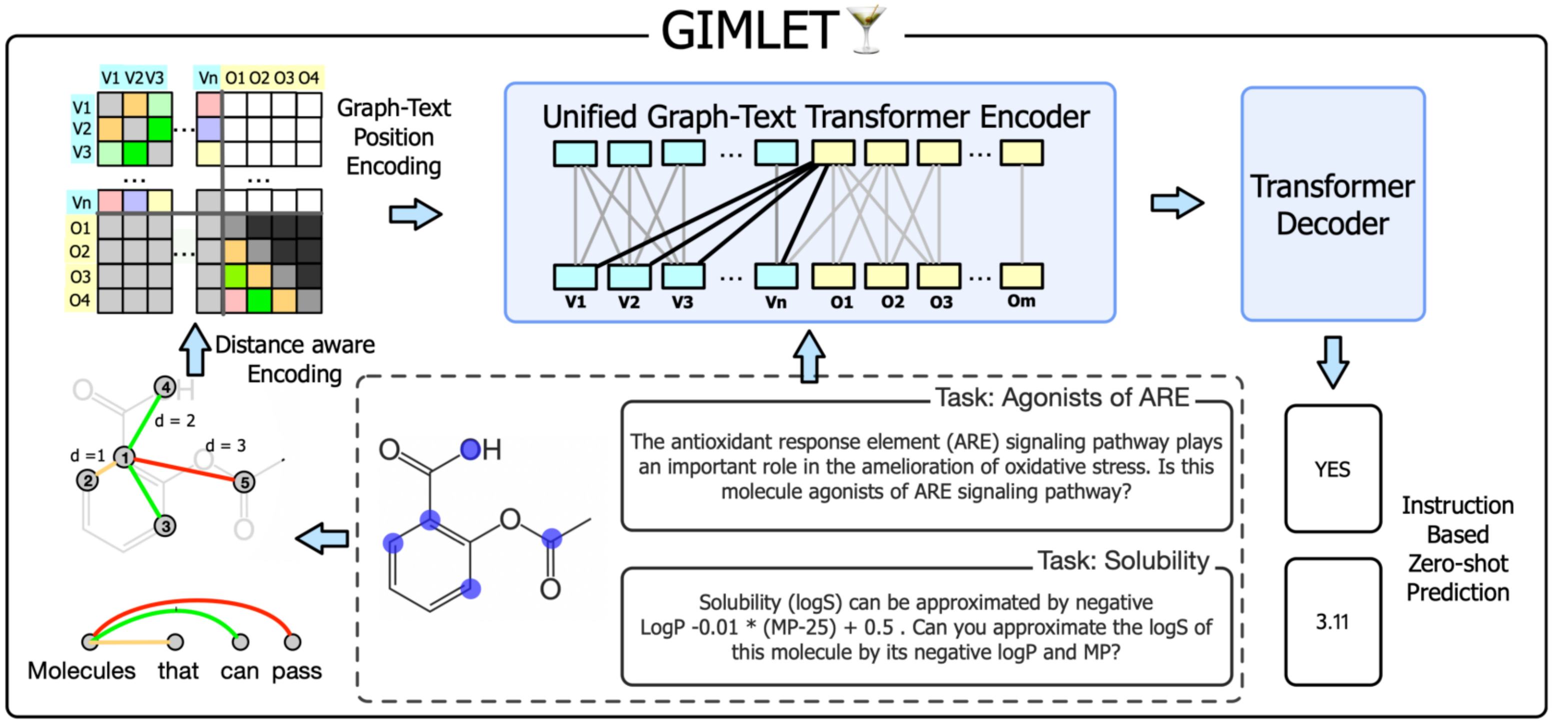
- Graph-to-Token
  - Tokenize graph information to align it with LLM
- Graph-to-text
  - Describe graph information using natural language



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

Graph-to-Token: GIMLET

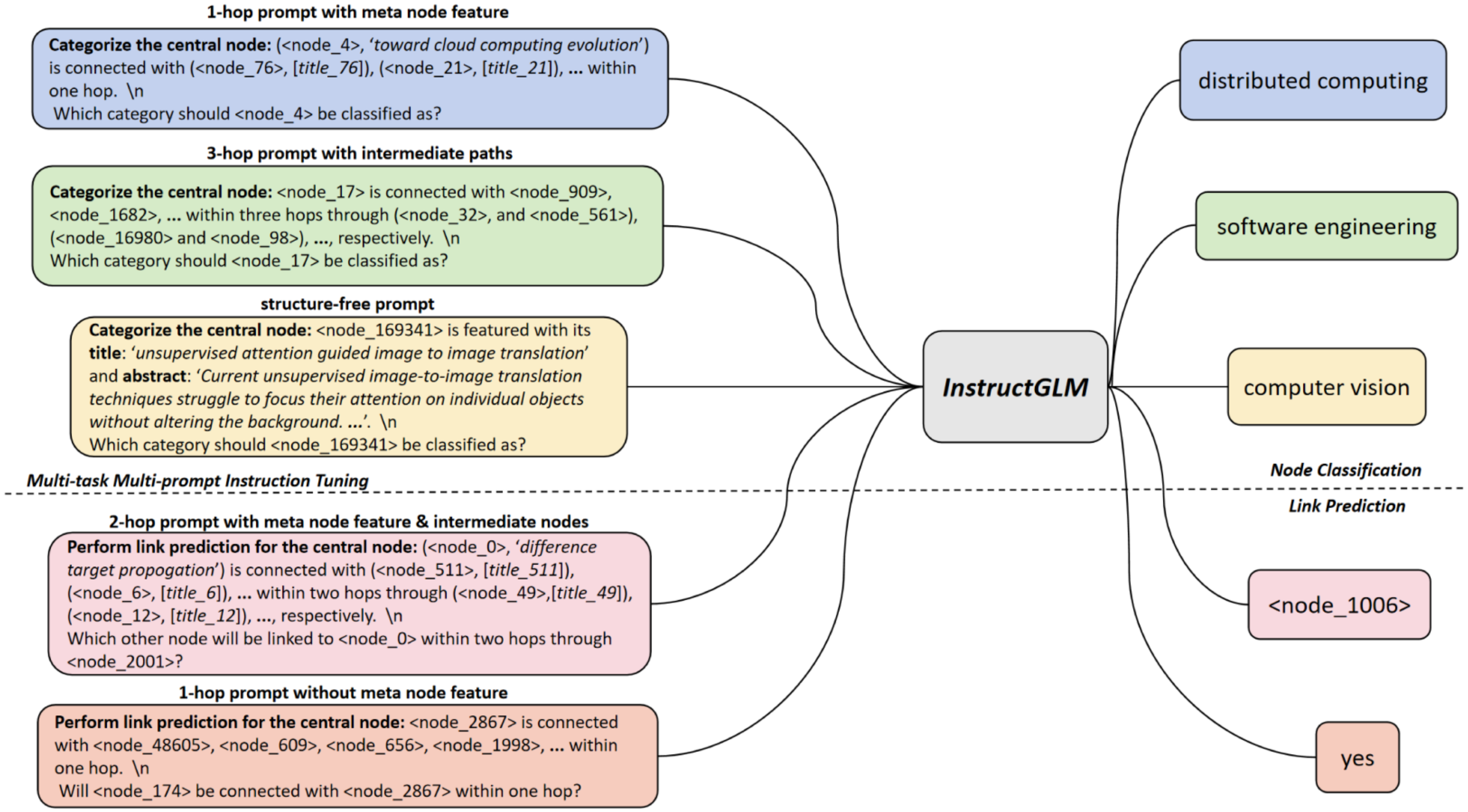
- Integrating graph data with textual data
- Encoding the graph's structural information



Zhao, et al. "GIMLET: A unified graph-text model for instruction-based molecule zero-shot learning." *NeurIPS'23.*

Graph-to-Token: InstructGLM

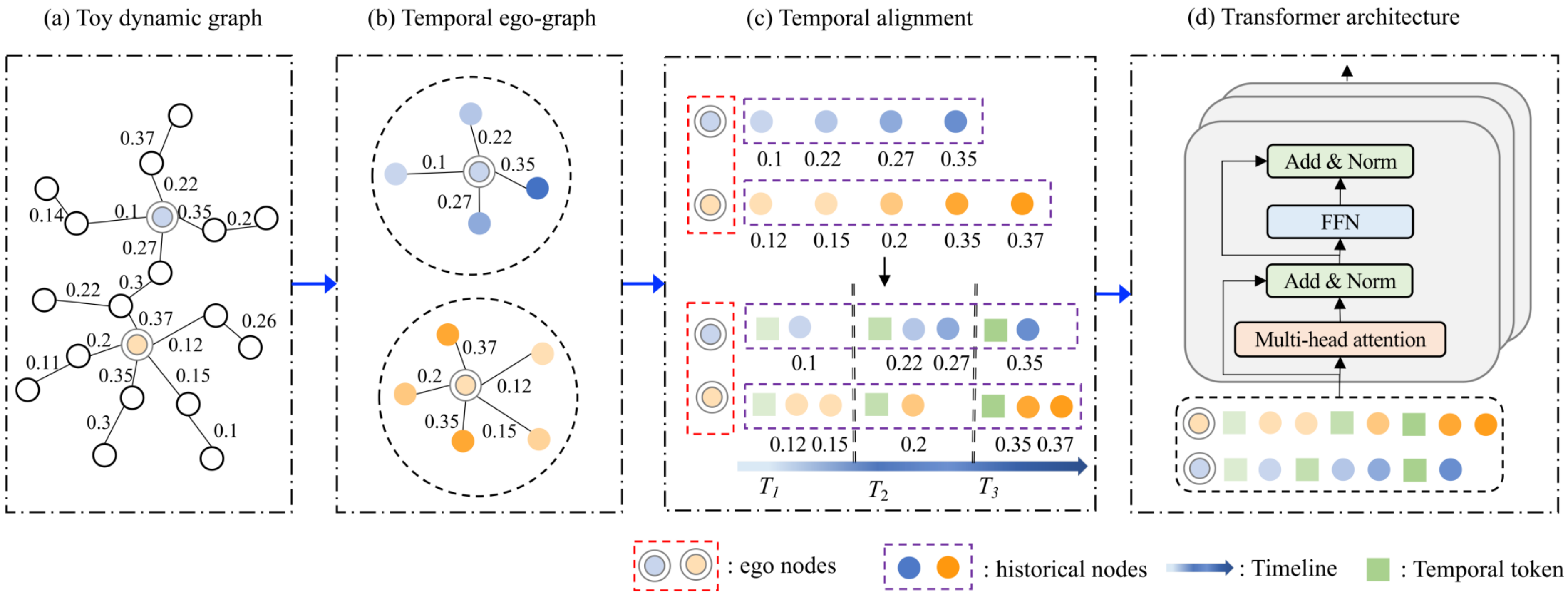
- Expand the vocabulary of the LLM by graph node features



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

Graph-to-Token: SimpleDyG

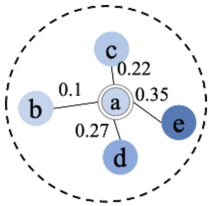
- Transformer-based approach for dynamic graphs
- Map a dynamic graph into a set of sequences



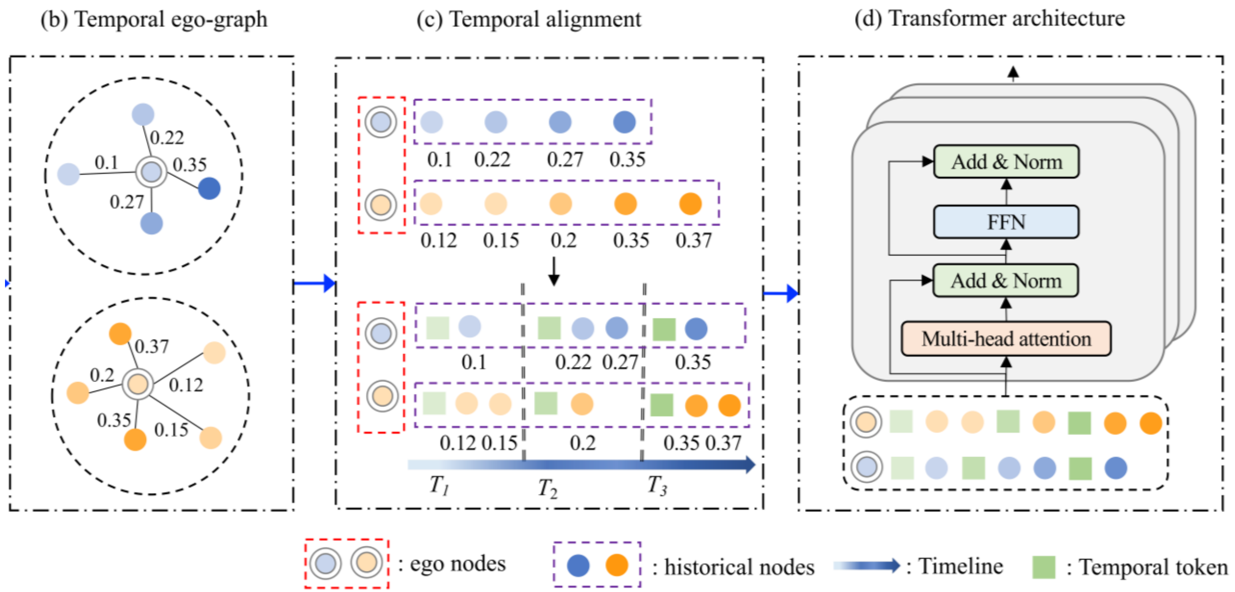
Wu, et al. "On the Feasibility of Simple Transformer for Dynamic Graph Modeling." *WWW'24*.

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:

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

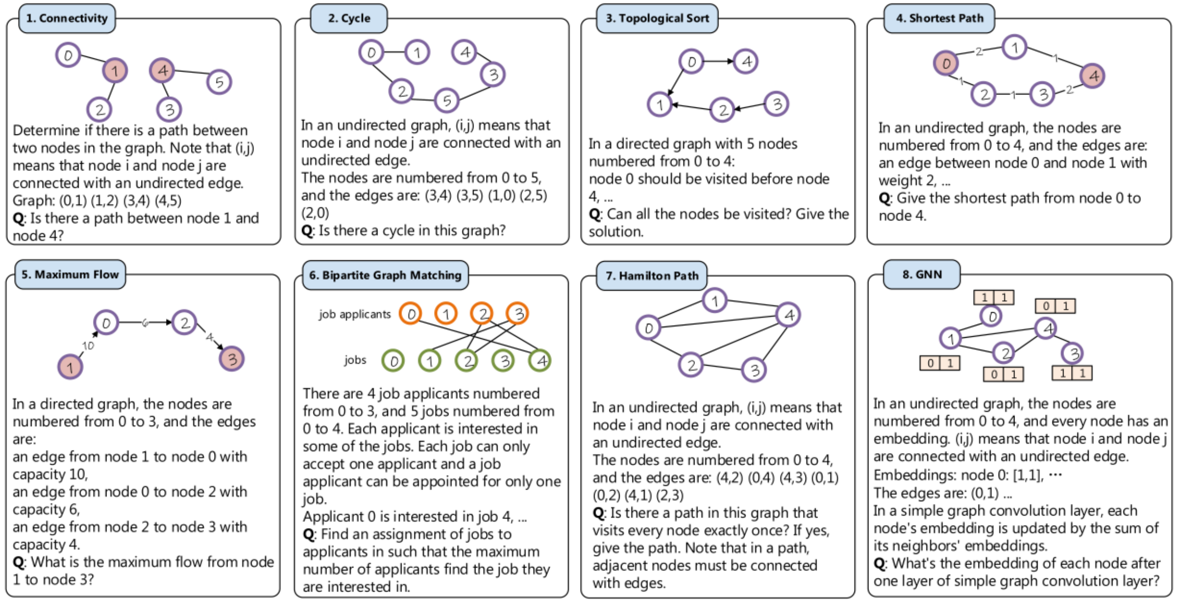
$$y_i' = \langle |pred| \rangle \langle |time4| \rangle S_i^4 \langle |endofpred| \rangle$$

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

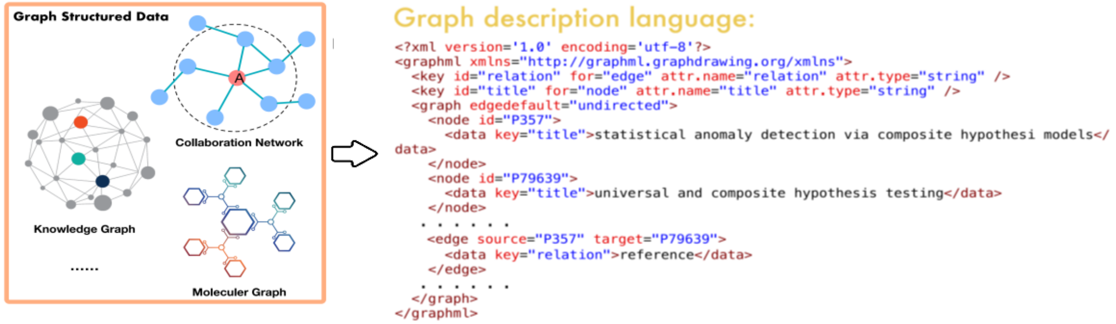
Graph-to-text

- ❑ Describe graph information for variours graphs and tasks

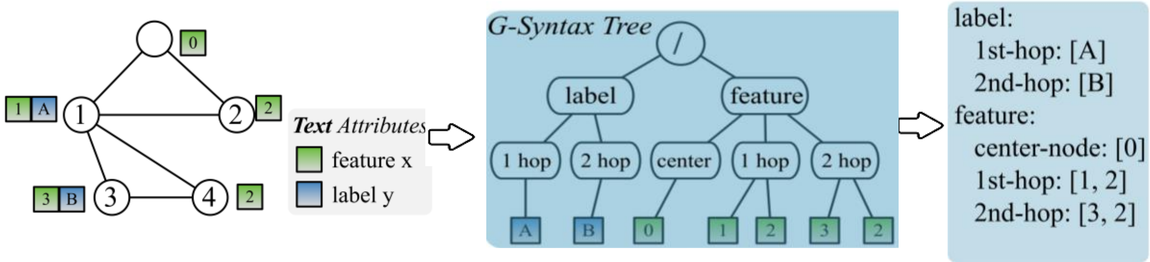
➢Node/edge list, graph properties



➢Graph description language



➢Graph-Syntax Tree



Wang, et al. "Can language models solve graph problems in natural language?." *NeurIPS'23.*

Guo, et al. "GPT4Graph: Can large language models understand graph structured data? an empirical evaluation and benchmarking." *CoRR'23.*

Zhao, et al. "GraphText: Graph reasoning in text space." *CoRR'23.*

LLM-based Models

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

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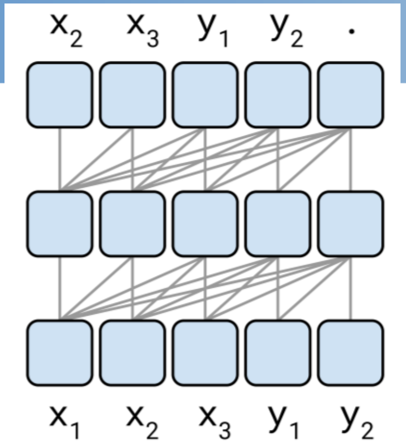
Table 3. Details of approaches involved as LLM based models

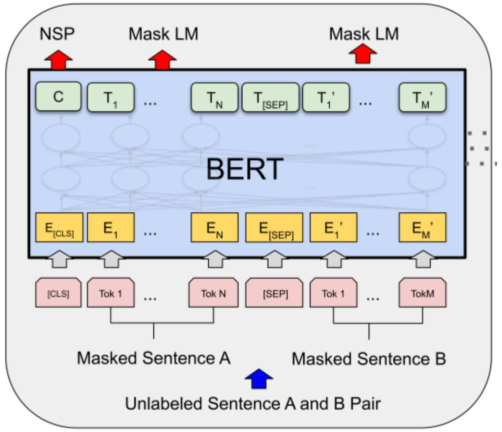
Pre-training

- ❑ Language Modeling (LM)
  - ➢ LLaMA, GPT-3...



- ❑ Masked Language Modeling (MLM)
  - ➢ BERT, T5...
  - ➢ Replace the word with the [MASK] token

    e.g., `my dog is hairy` → `my dog is [MASK]`



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

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- ❑ Pre-training
- ❑ **Adaptation**

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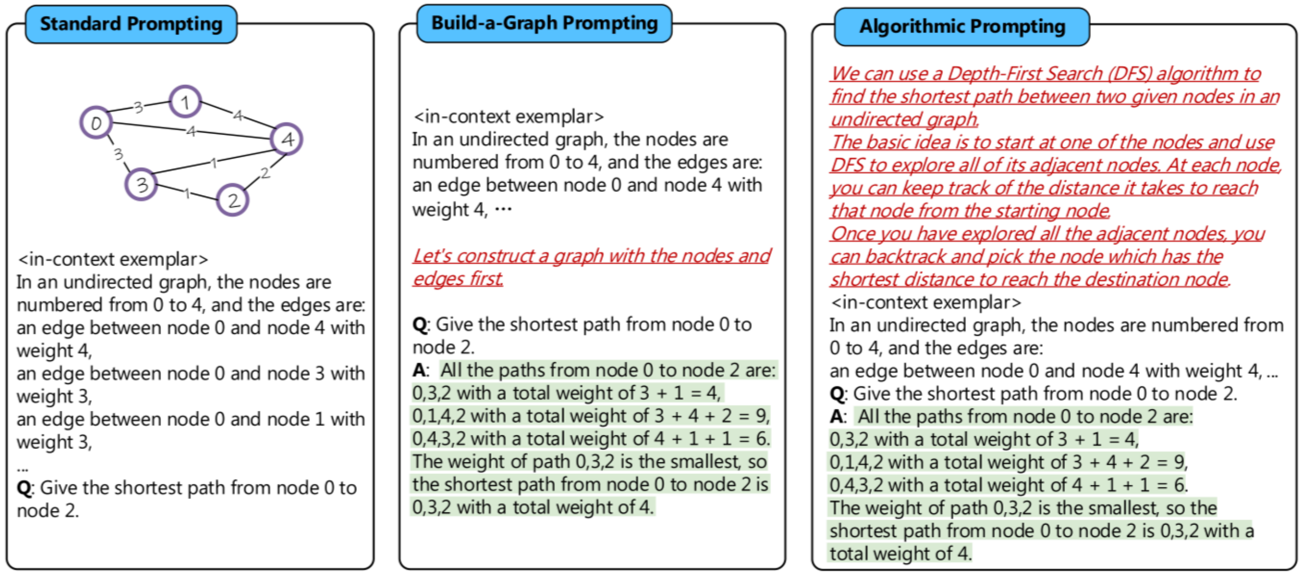
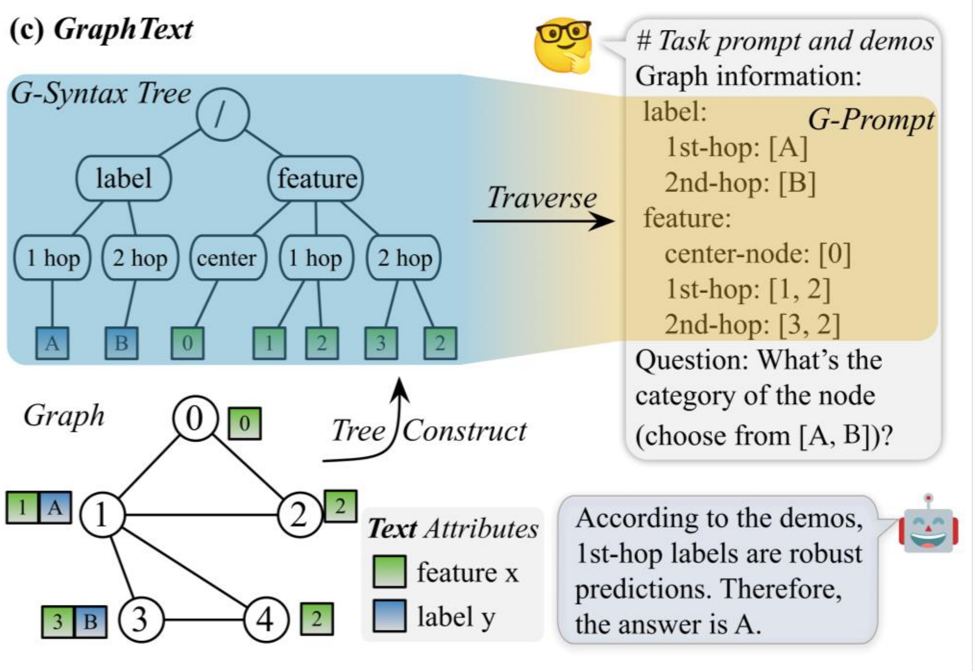
Adaptation

- ❑ Manual Prompting: Graph information, task descriptions
- ❑ Automatic Prompting: LLMs--> generate the context





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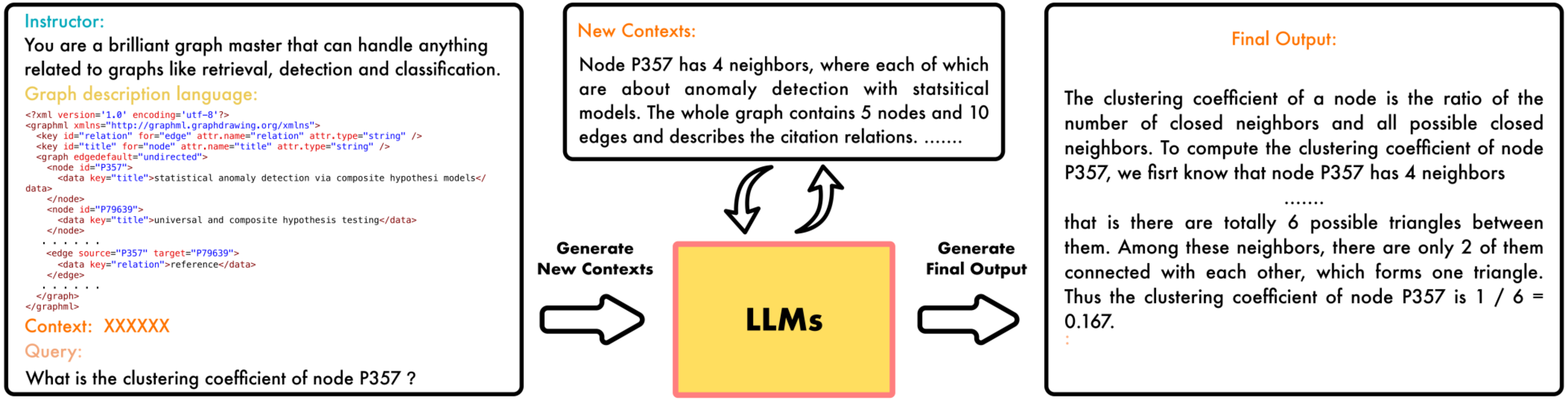
Zhao, et al. "GraphText: Graph reasoning in text space." *CoRR'23*

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." *CoRR'23*

Chen, et al. "Exploring the potential of large language models (llms) in learning on graphs." *ACM SIGKDD Explorations Newsletter 2024*

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

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
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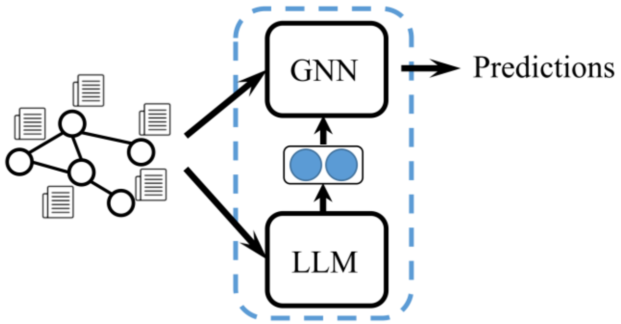
MoMu [109]	Symmetric	MLM + GTCL	Parameter-Efficient FT
MoleculeSTM [73]	Symmetric	MLM + GTCL	Parameter-Efficient FT
CLAMP [103]	Symmetric	MLM + GTCL	Parameter-Efficient FT
Graph-Toolformer [165]	LLM-centric	LM	Tuning-free Prompting + Vanilla FT

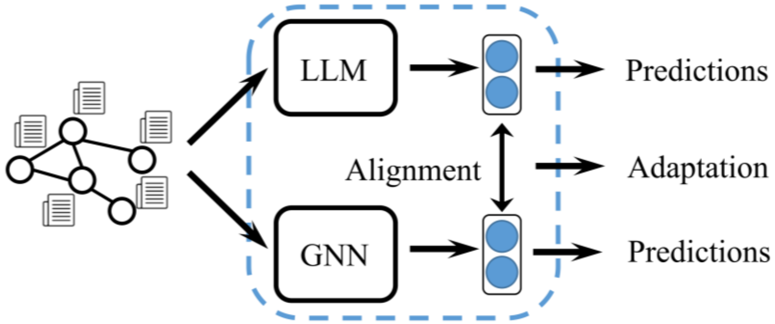
Table 4. Details of approaches involved as GNN+LLM based models

Backbone Architectures

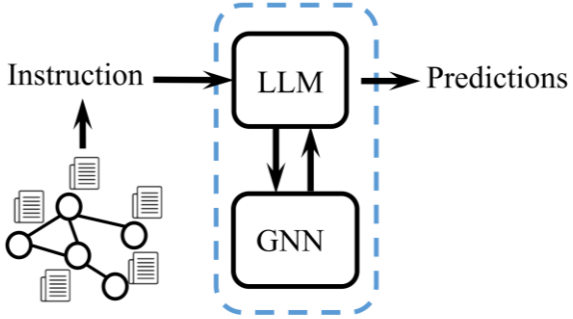
- GNN-centric Methods
  - LLMs extract node features from raw data; GNNs make predictions
- Symmetric Methods
  - Align the embeddings of GNN and LLM
- LLM-centric Methods
  - Utilize GNNs to enhance the performance of LLM



(a) GNN-centric methods.



(b) Symmetric methods.

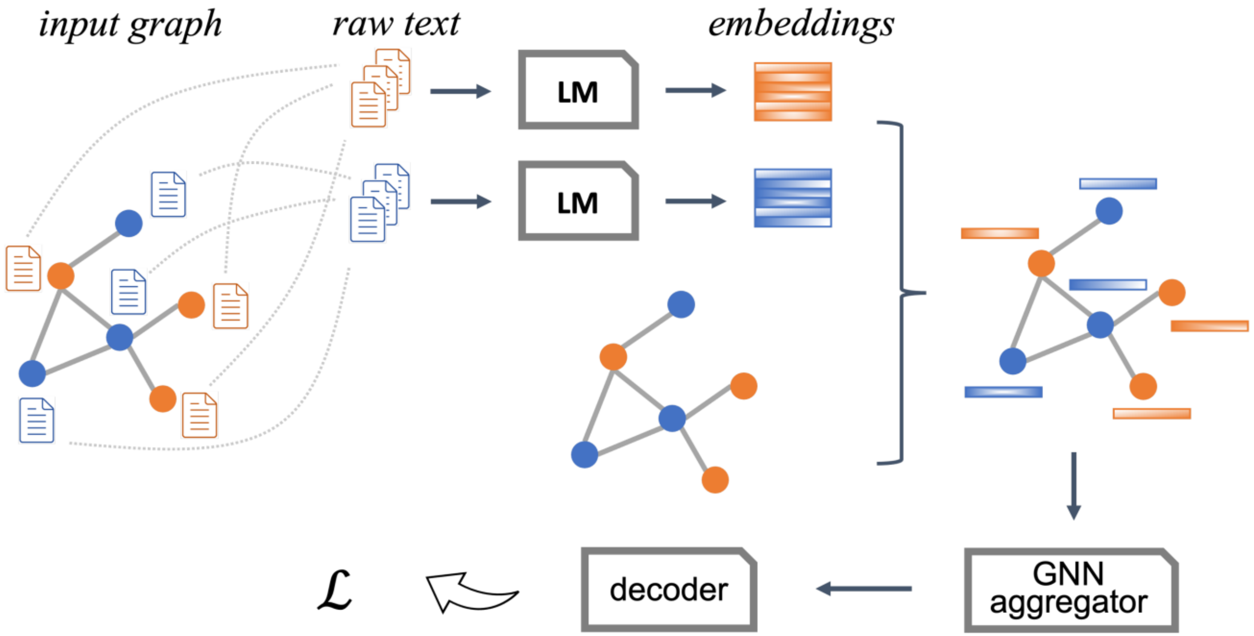


(c) LLM-centric methods.

GNN-centric Methods: GaLM

- The backbone model:

  Raw text → LMs → GNN aggregator → decoder



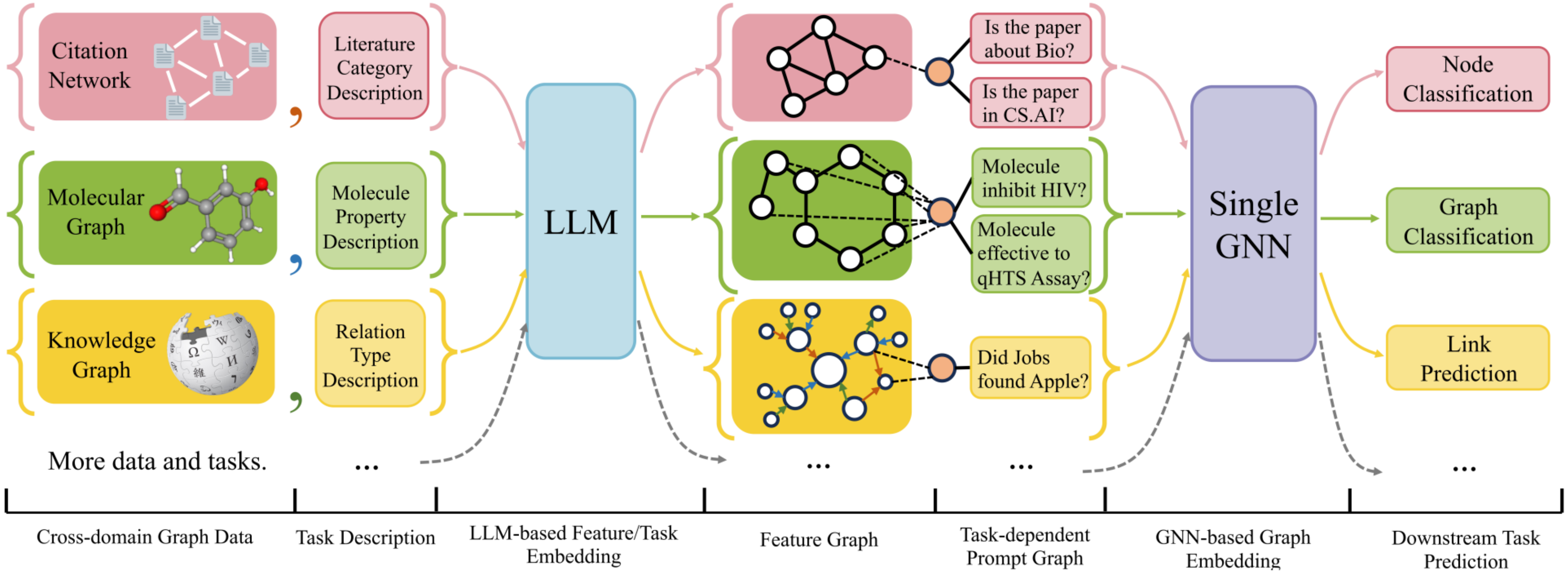
Xie, et al. "Graph-aware language model pre-training on a large graph corpus can help multiple graph applications." *KDD'23*.

GNN-centric Methods: One for all

❑ The backbone model:

Text-attributed graph
Task description

LLMs → Prompted graph → GNN → Downstream tasks

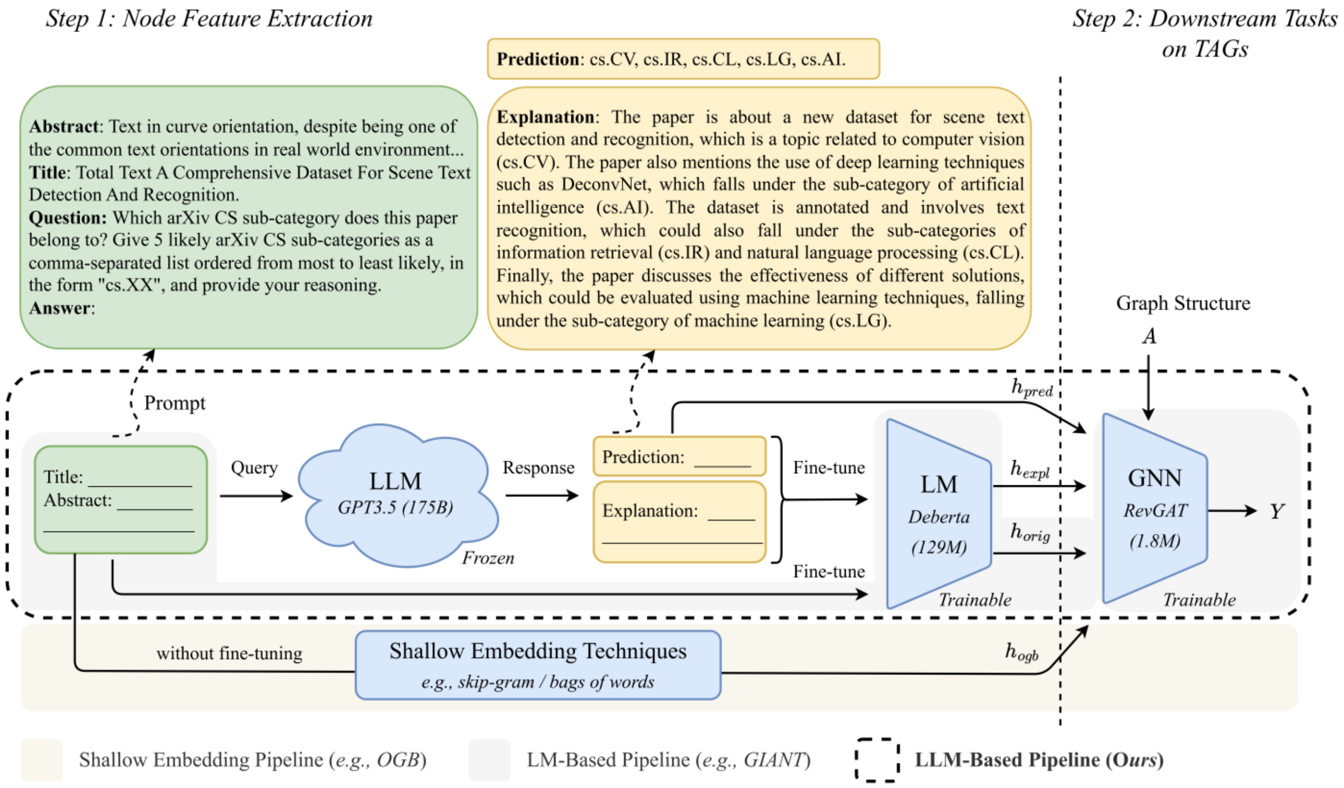


Liu, et al. "One for all: Towards training one graph model for all classification tasks." *ICLR'24*

GNN-centric Methods: TAPE

- The backbone model:

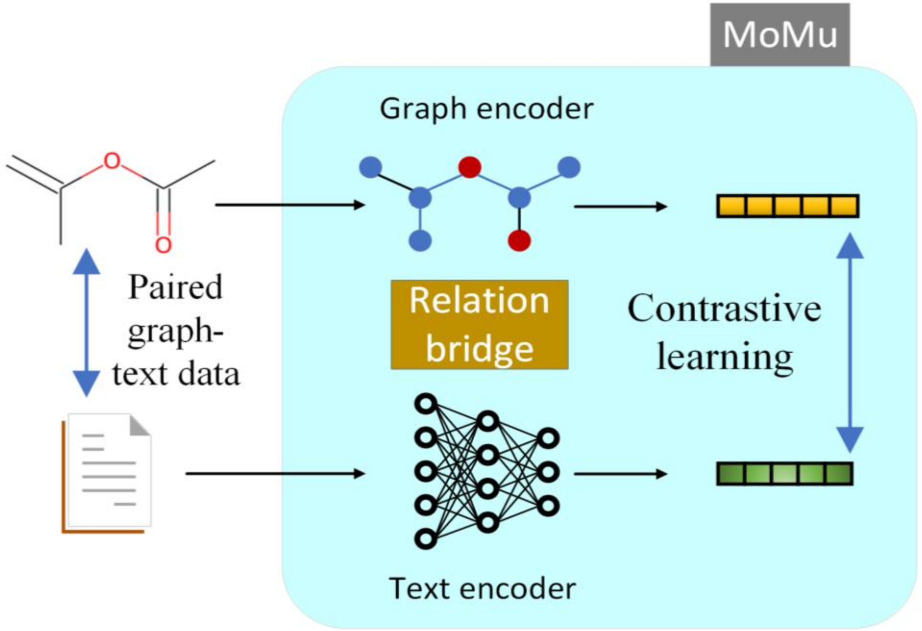
Textual attributes → LLM → Prediction & Explanation → Fine-tune LM → Node features → GNN

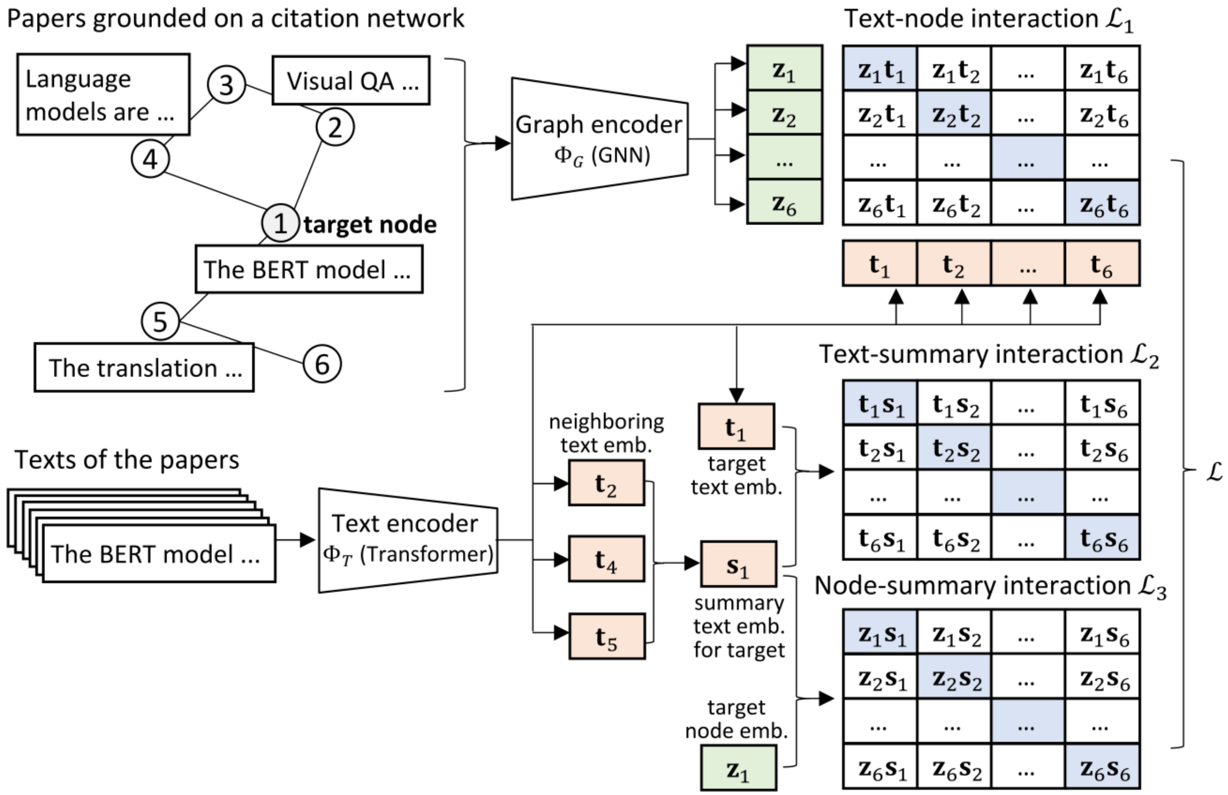


He, et al. "Harnessing explanations: LLM-to-LM interpreter for enhanced text-attributed graph representation learning." *ICLR'24*

Symmetric Methods: MoMu, G2P2

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





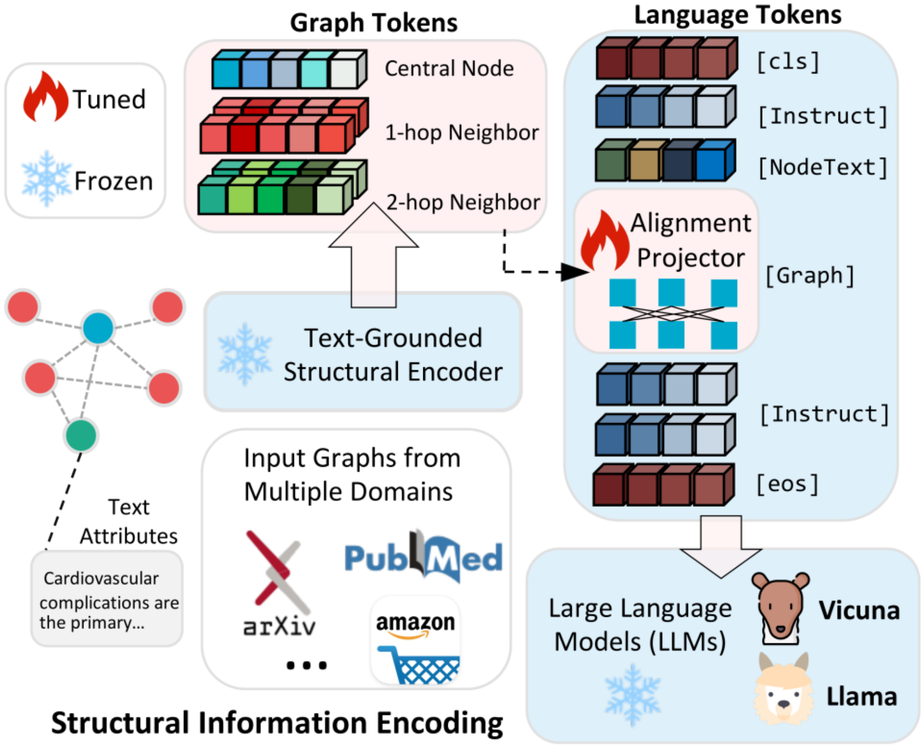
Su, et al. "A molecular multimodal foundation model associating molecule graphs with natural language." *CoRR'22*.

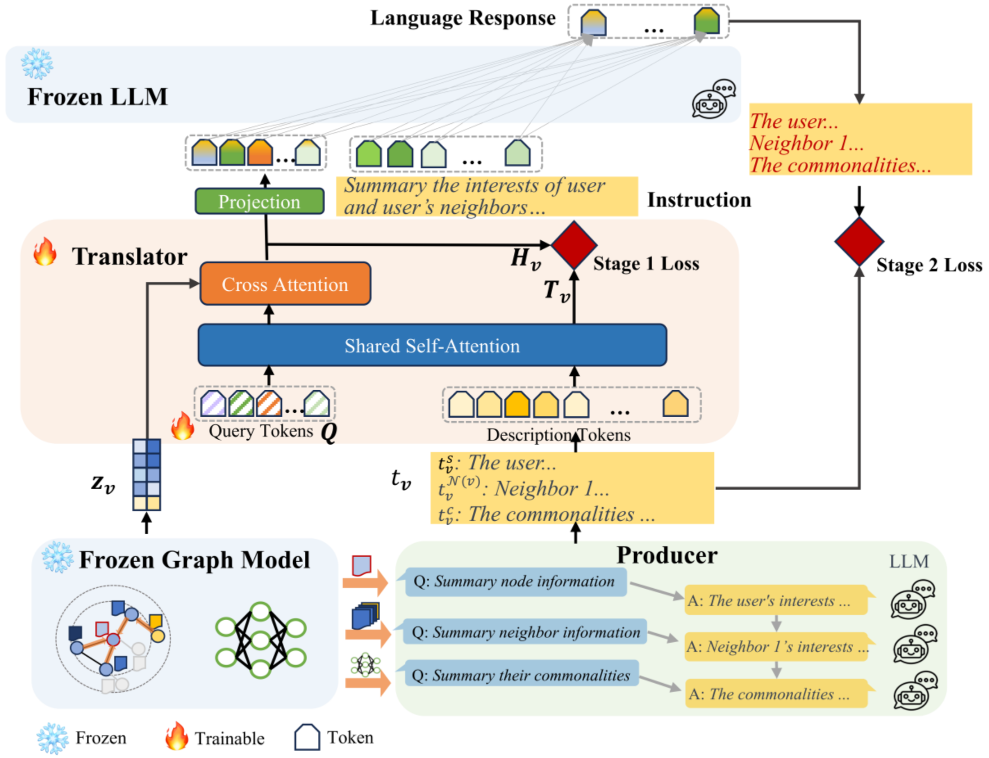
Wen, et al. "Augmenting low-resource text classification with graph-grounded pre-training and prompting." *SIGIR'23*.

LLM-centric Methods: GraphGPT, GraphTranslator

- The backbone model:

  Graph → GNN → Projection → LLM





Tang, et al. "GraphGPT: Graph instruction tuning for large language models." *SIGIR'24*

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

GNN+LLM based Models

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

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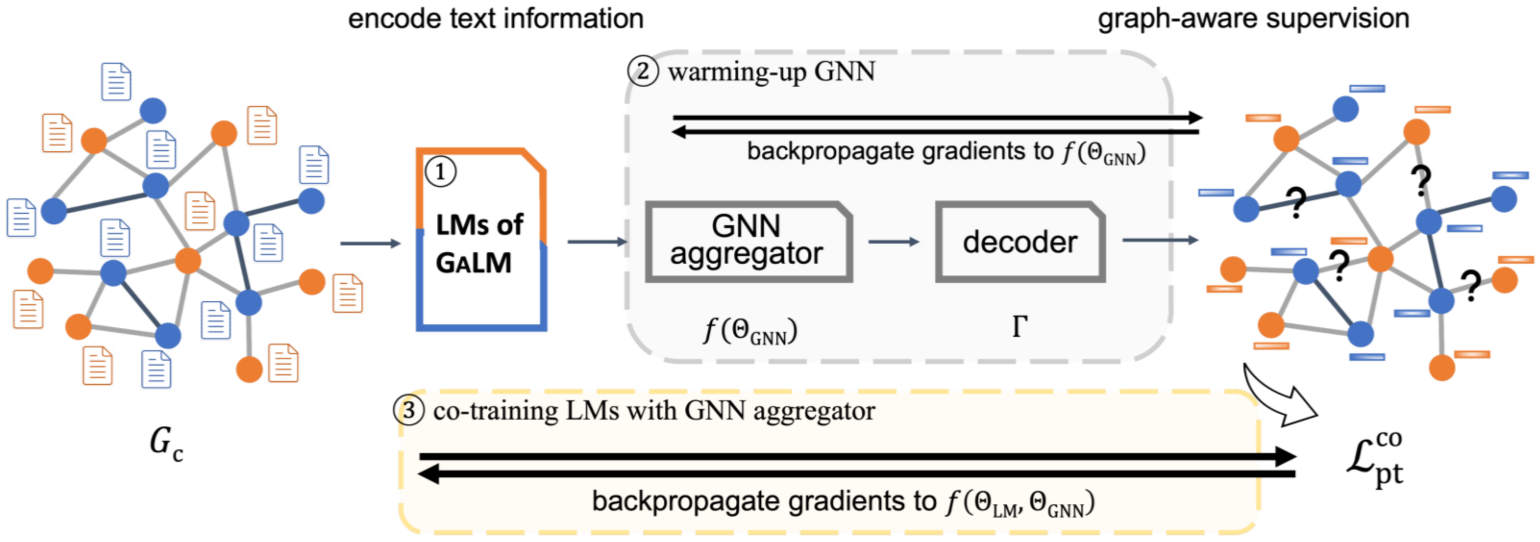
Table 4. Details of approaches involved as GNN+LLM based models

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

- GaLM (Graph-aware Language Model pre-training):
  - Fine-tuning existing general LMs by graph-aware supervision
  - Warming up the GNN aggregator by fixing the pre-trained LMs
  - Co-training GNN+LMs



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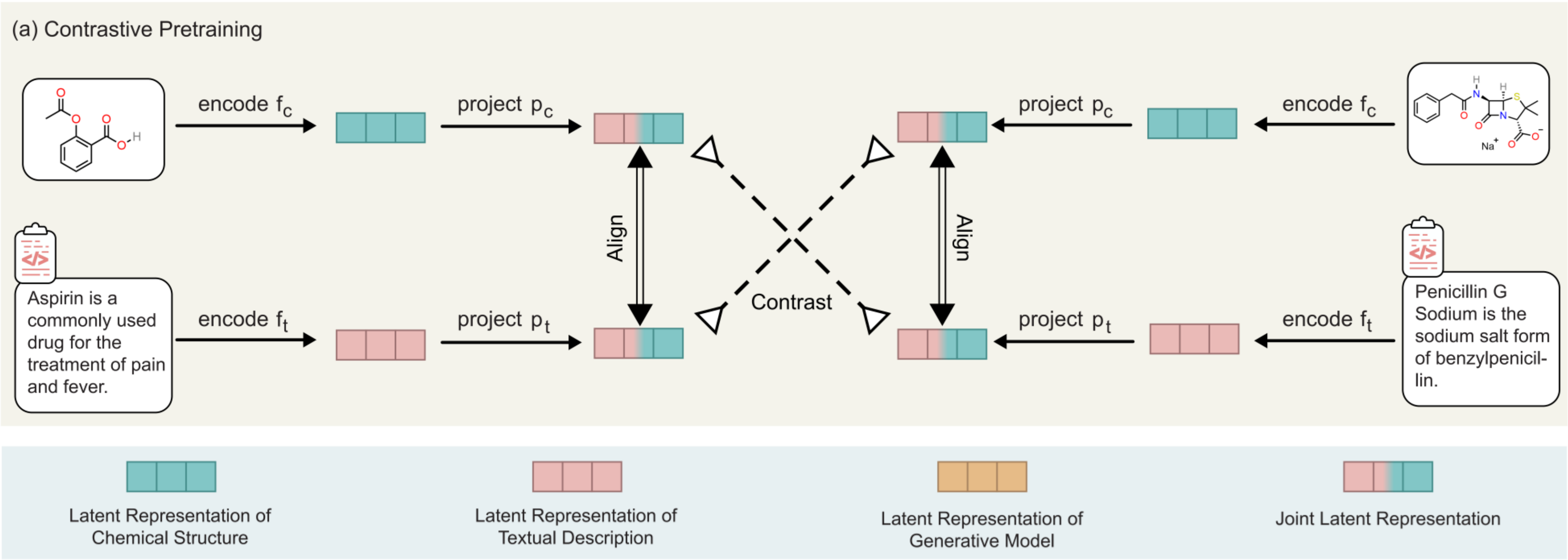
Alignment-based: MoleculeSTM

❑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

- Dual encoders
- Three kinds of alignments
  - Text-Node: L1
  - Text summary-Text: L2
  - Text summary-Node: L3
    - Text-summary: text of neighbors

$$\mathbf{s}_i = \frac{1}{|\mathcal{N}_i|} \sum_{j \in \mathcal{N}_i} \mathbf{t}_j$$

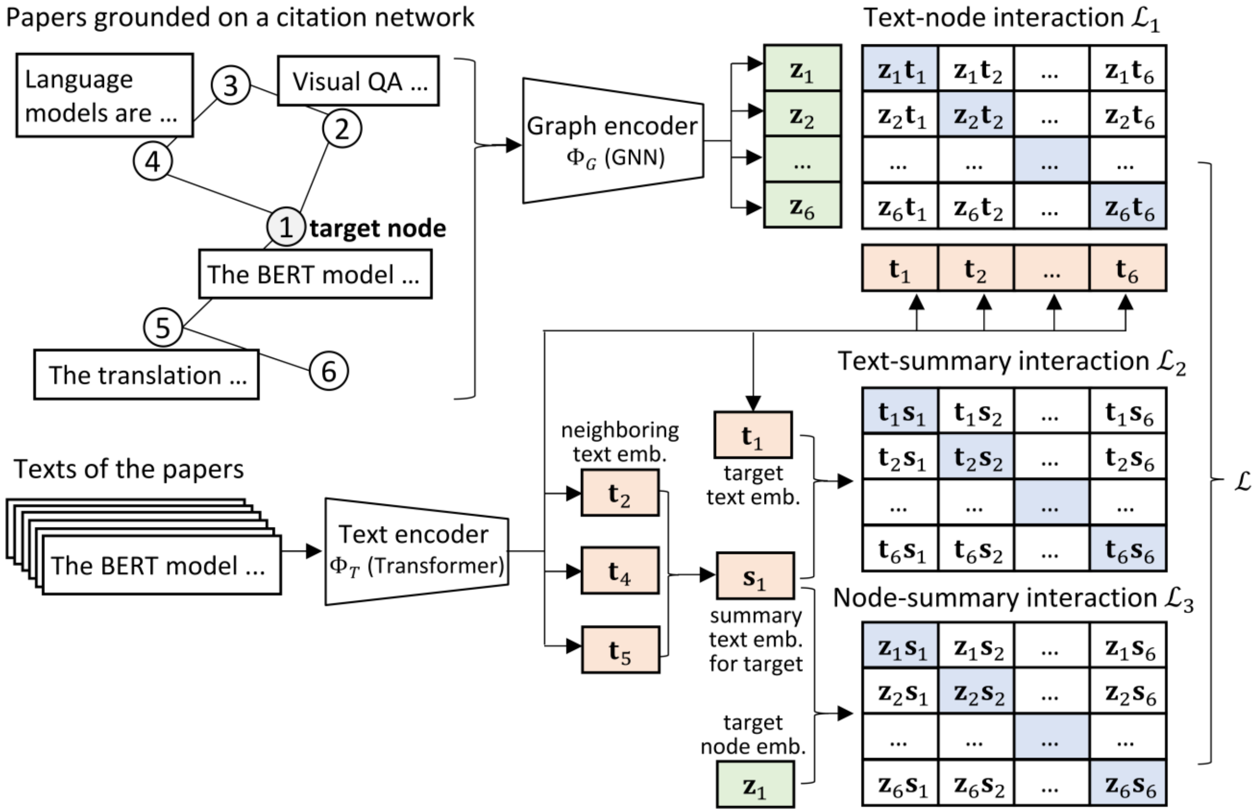


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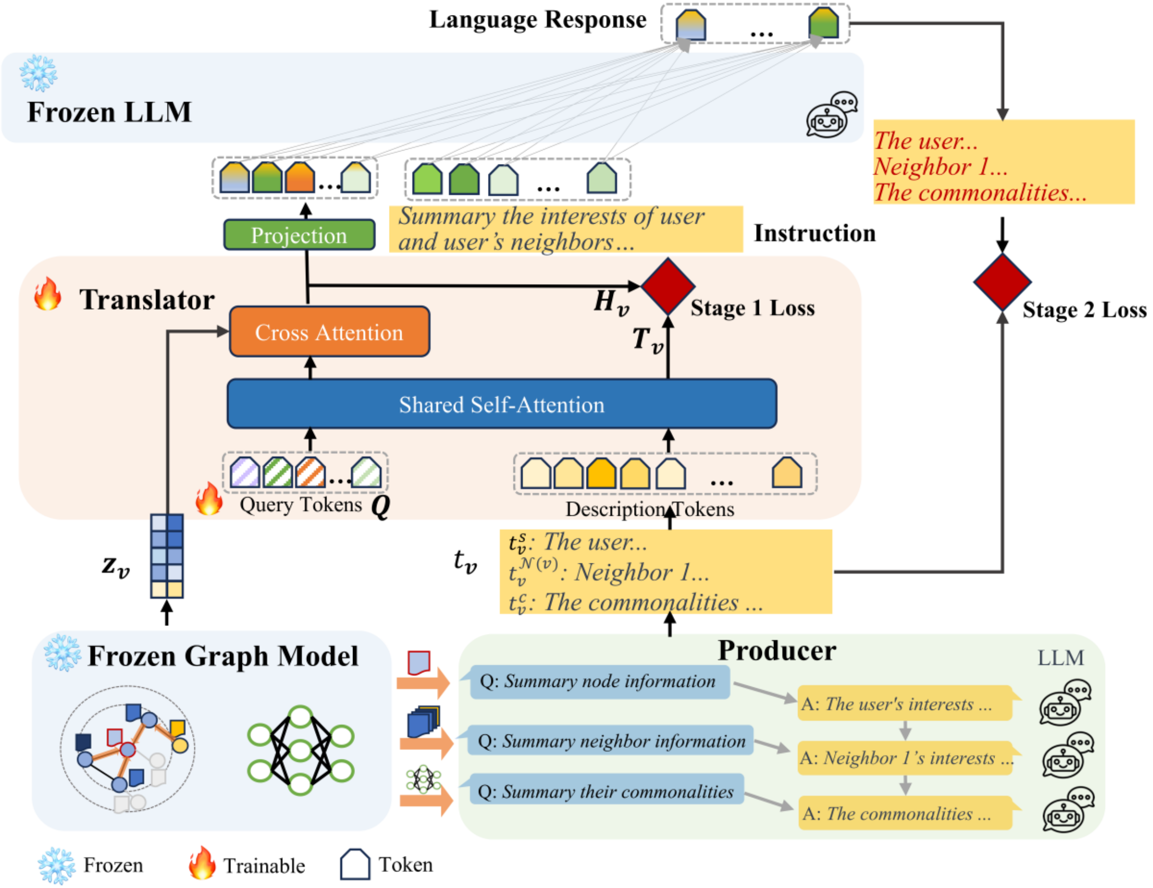
Table 4. Details of approaches involved as GNN+LLM based models

Adaptation

- Fine-tuning
  - Vanilla tuning: tune all the parameters
    - computationally intensive, resource-demanding
  - Parameter-efficient fine-tuning (PEFT): tune a subset of parameters
    - more efficient, resource-friendly
- Prompt-Tuning: design and tune external prompts

PEFT: GraphTranslator

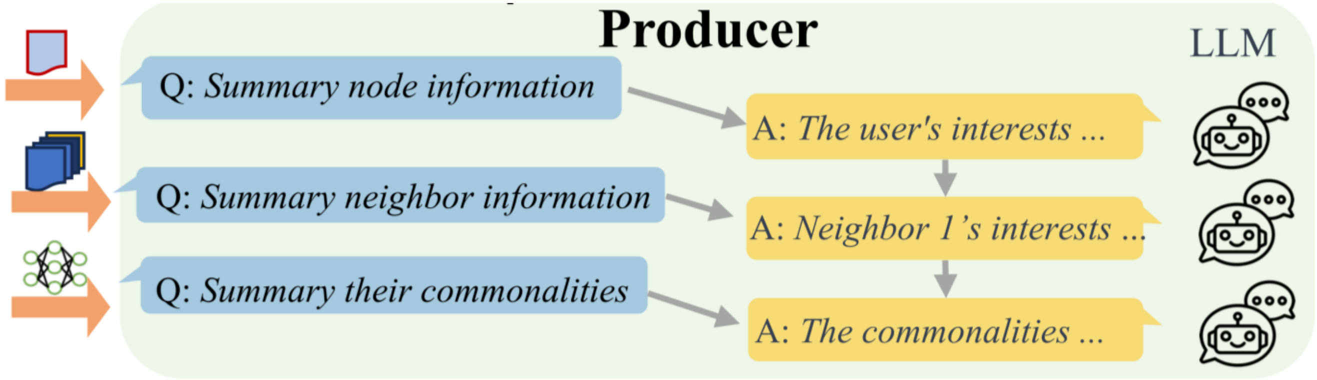
- ❑ Frozen:
  - ➢ Graph Model
  - ➢ Large Language Model
- ❑ Tunable:
  - ➢ Producer Module
    - ▪ Construct alignment data
  - ➢ Translator Module
    - ▪ Convert node representations into tokens for LLM prediction



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

PEFT: GraphTranslator

- Producer:
  - “Chain of Thought” (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?

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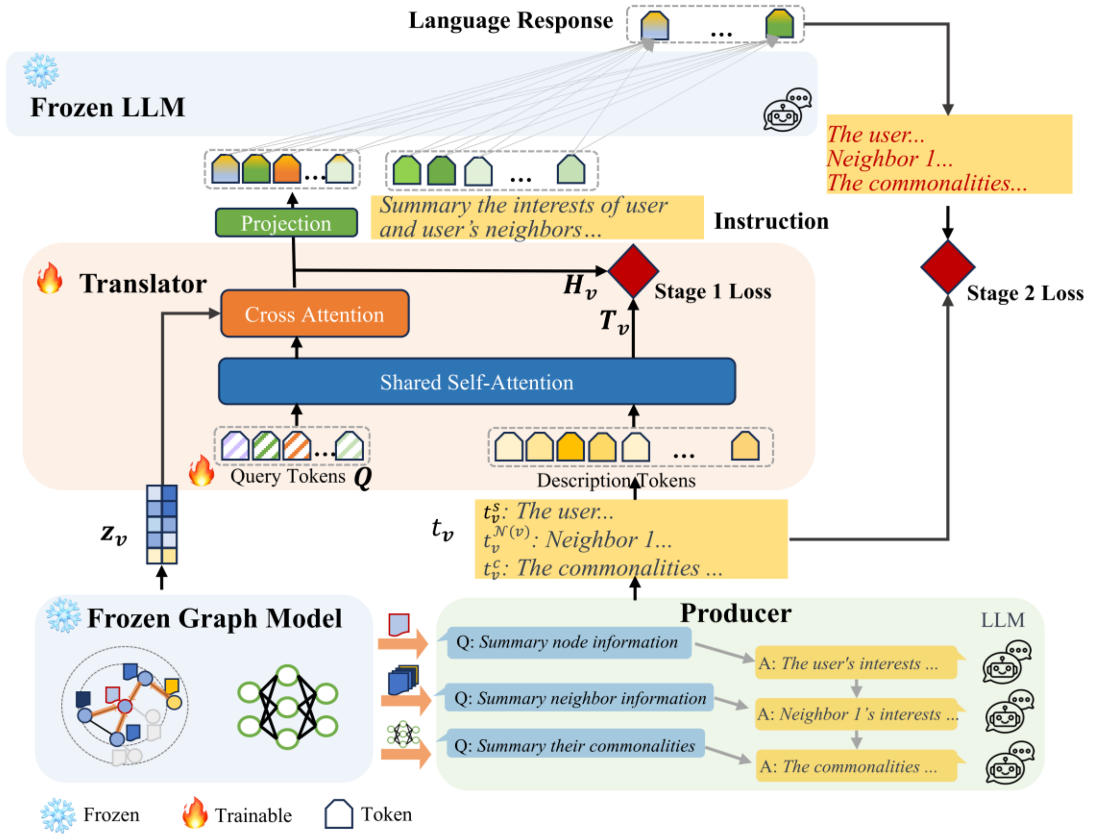
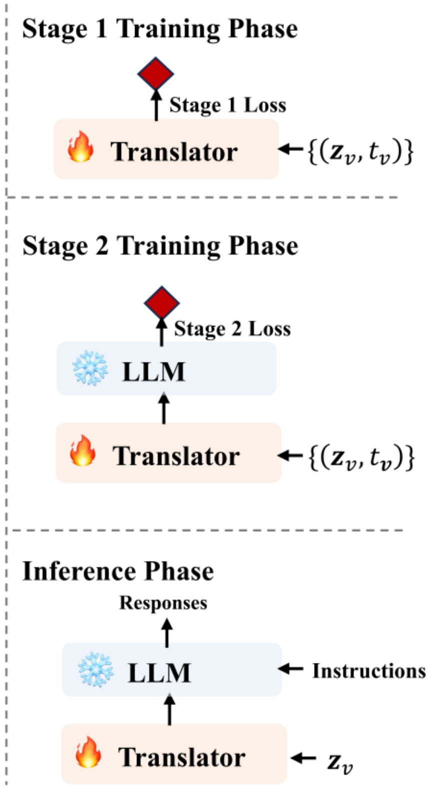
PEFT: GraphTranslator

- Training: Only fine-tune Translator and Projection





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

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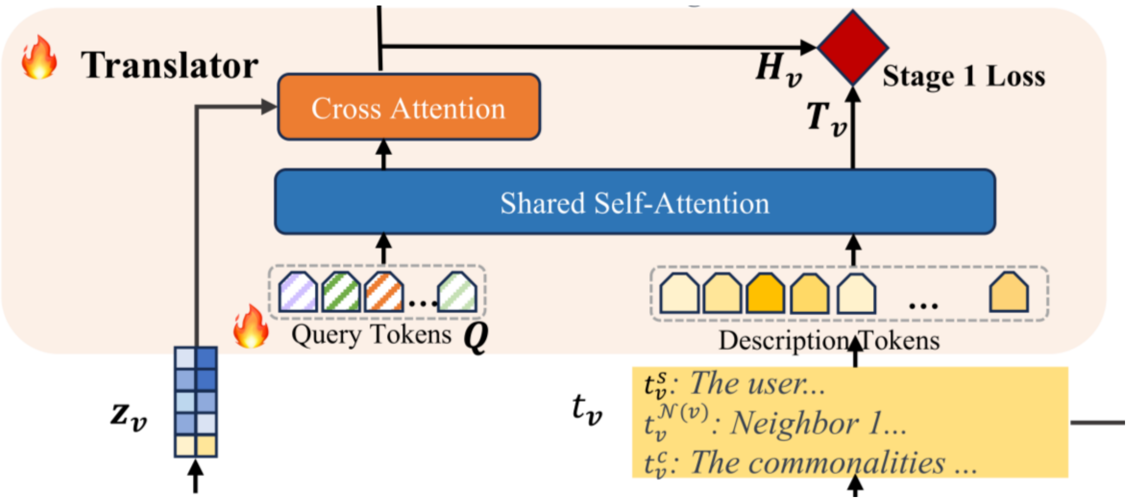
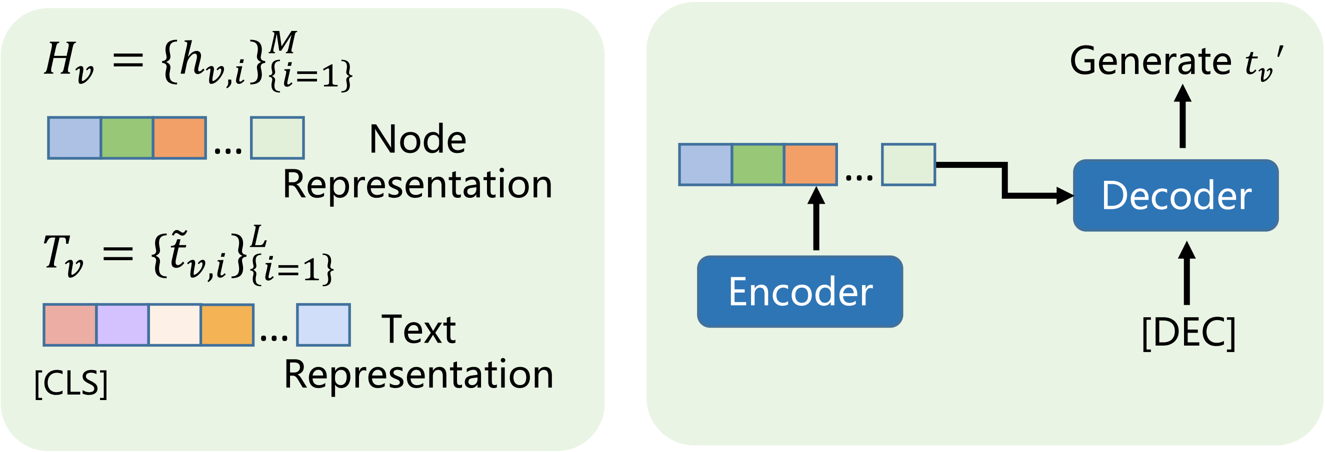
PEFT: GraphTranslator

❑ Training: Stage 1



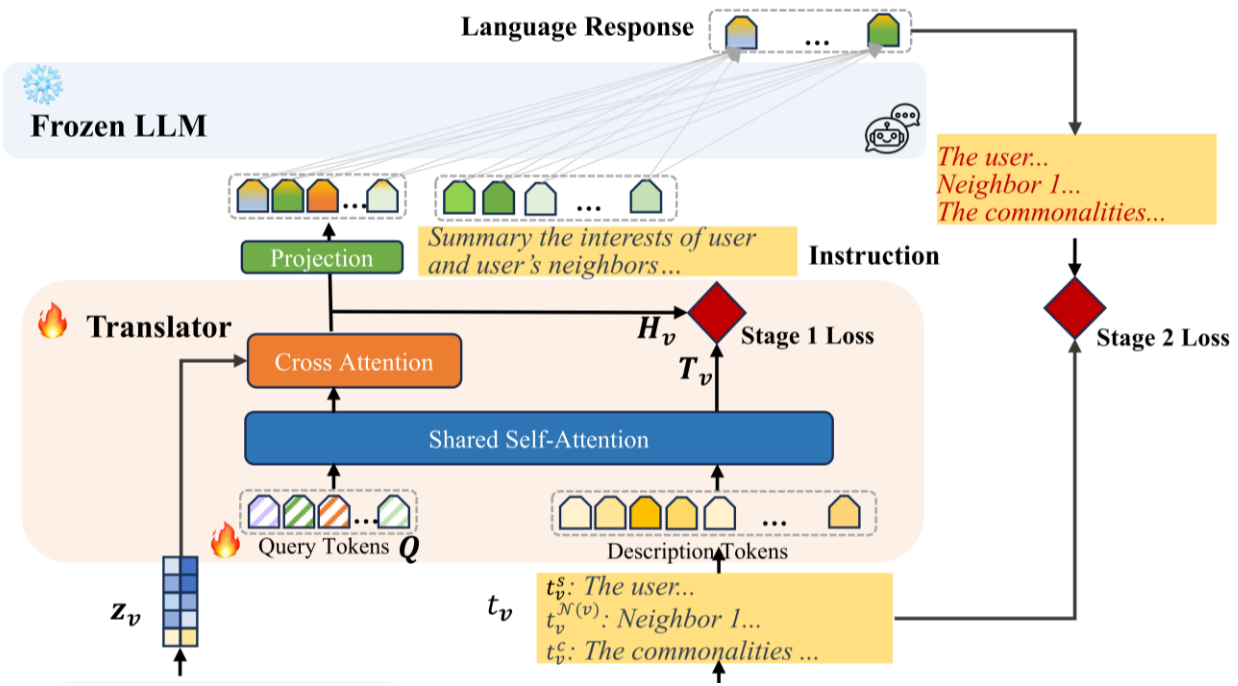


- ➢ Contrastive Objective
  - Node ↔ Text
  - High-level alignment
- ➢ Matching Objective
  - Node ↔ Text
  - Fine-grained alignment
- ➢ Generation Objective
  - Node → Text
  - Replace the [CLS] token with a new [DEC] token as the first text token to signal the decoding task

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

PEFT: GraphTranslator

❑ Training: Stage 2

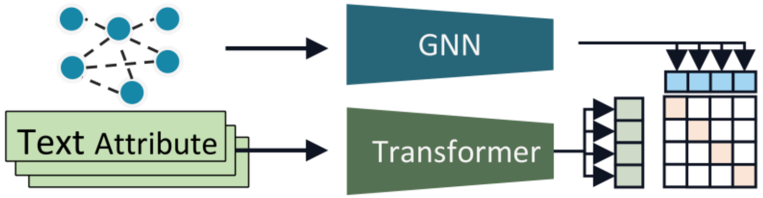


- Projection:
  - A linear layer: project H_v to token representation space of LLM
- Concatenate:
  - Connect the projected representation with the human instruction and feed into LLM
- Fine-tune Translator
  - Alignn the response text of LLM with the actual descriptive text

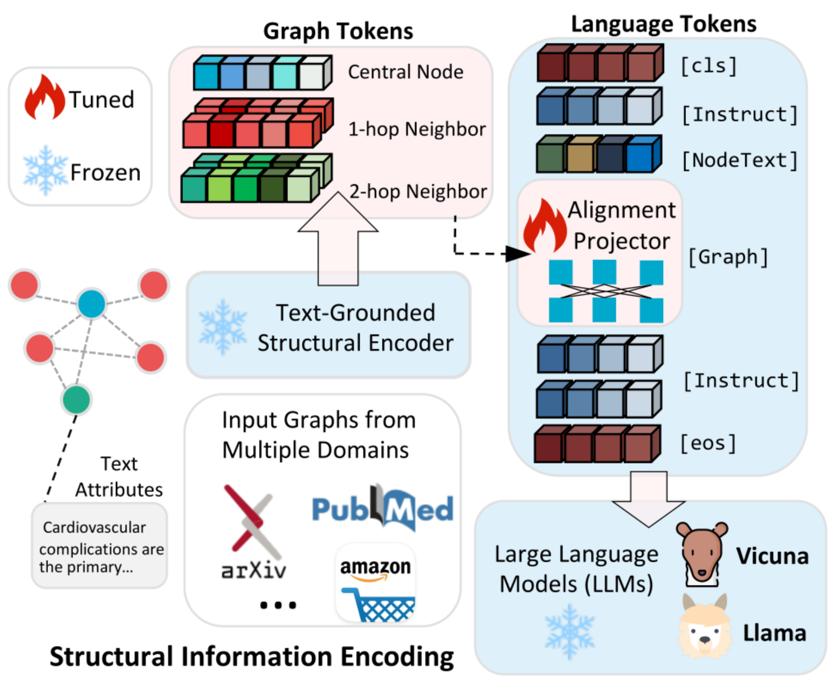
Zhang, et al. "GraphTranslator: Aligning Graph Model to Large Language Model for Open-ended Tasks." WWW’24

PEFT: GraphGPT

- ❑ Graph: Text-Grounded Structural Encoder



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



Graph Information: <graph>: **Central Node:** 68442, **Edge index:** [[…src node…],[…dst node…]], **Node list:** […] **Graph Matching**
Human Question: Given a sequence of graph tokens **<graph>** that constitute a subgraph of a citation graph, …. Here is a list of paper titles: 1. … 2. …, please reorder the list of papers according to the order of graph tokens.
GraphGPT Response: Based on the given graph tokens and the list of paper titles, we obtain the matching of graph tokens and papers: Graph token 1 corresponds to smt based induction methods for timed systems. Graph token 2 corresponds to …

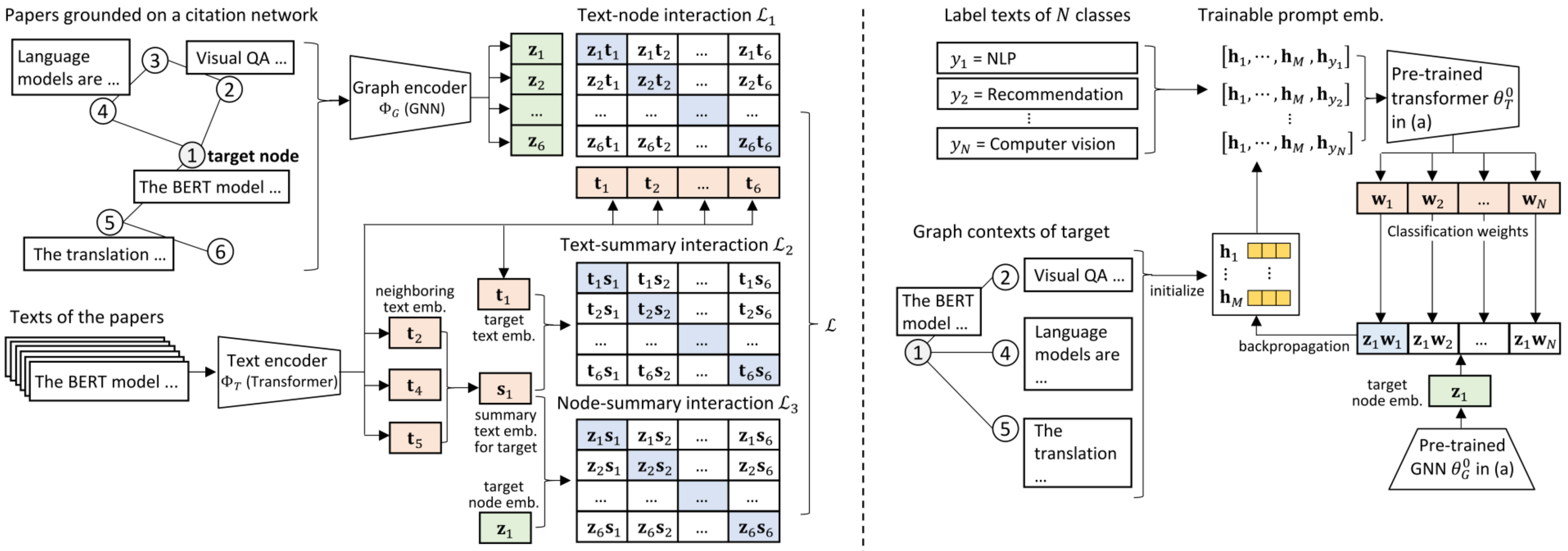
Graph Information: <graph>: **Central Node:** 2, **Edge index:** [[…src node…],[…dst node…]], **Node list:** […] **Node Classification**
Human Question: Given a citation graph: **<graph>** where the 0th node is the target paper, with the following information: Abstract: … Title: … Question: Which arXiv CS sub-category does this paper belong to? …
GraphGPT Response: cs.IT, cs.LG, cs.SP, cs.CV, cs.NA. The paper discusses the Restricted Isometry …. So, it is likely to belong to cs.IT…

Graph Information: <graph>: **Central Node 1:** 8471, **Edge index 1:** [[…src node…],[…dst node…]], **Node list 1:** […] **Link Prediction**
<graph>: **Central Node 2:** 19368, **Edge index 2:** [[…src node…],[…dst node…]], **Node list 2:** […]
Human Question: Given a sequence of graph tokens: **<graph>** that constitute a subgraph of a citation graph, …. Abstract: … Titile: … and the other sequence of graph tokens: **<graph>**, … Abstract: … Title: …, are these two central nodes connected? Give me an answer of "yes" or "no".
GraphGPT Response: Yes, they are connected. Based on the first paper, …. And the second paper proposes ….

Tang, et al. "GraphGPT: Graph instruction tuning for large language models." *SIGIR'24*

Prompt-Tuning: G2P2

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



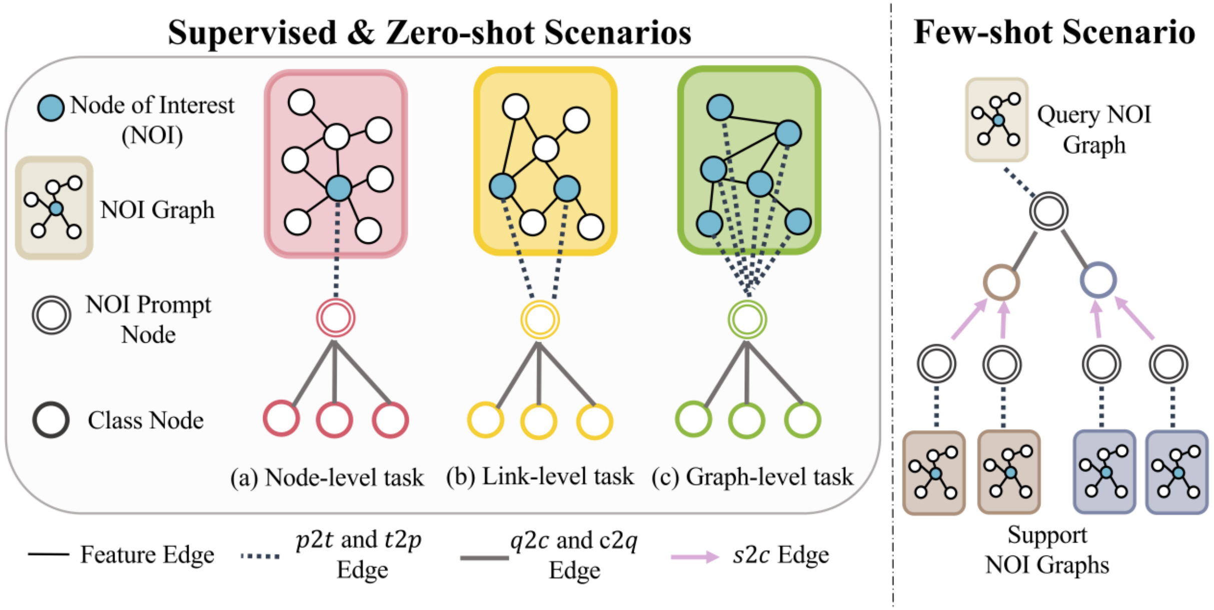
(a) Graph-grounded contrastive pre-training

(b) Graph-grounded prompt tuning (few-shot classification)

Wen, et al. "Augmenting low-resource text classification with graph-grounded pre-training and prompting." *SIGIR'23*.

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." *ICLR'24*.

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

- ➢ Focus on resolving LLMs' limitations: multi-hop reasoning, graph topology, and diverse graph data.
- ➢ Explore efficient training methods to manage the high computational costs and data requirements.
- ➢ Explore applications of GNN+LLM models in multimodal and cross-modal tasks.