

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 Architectures
- Pre-training
- Adaptation

□ GNN+LLM based Models

- Backbone Architectures
- Pre-training
- Adaptation

□ Summary and outlook

LLM-based Models

□ Backbone Architectures

□ 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
Graph4LLM[90]	Graph-to-text + BERT, DeBERTa, Sentence-BERT, GPTs, LLaMA	MLM,LM	Manual Prompt Tuning + Automatic Prompt Tuning

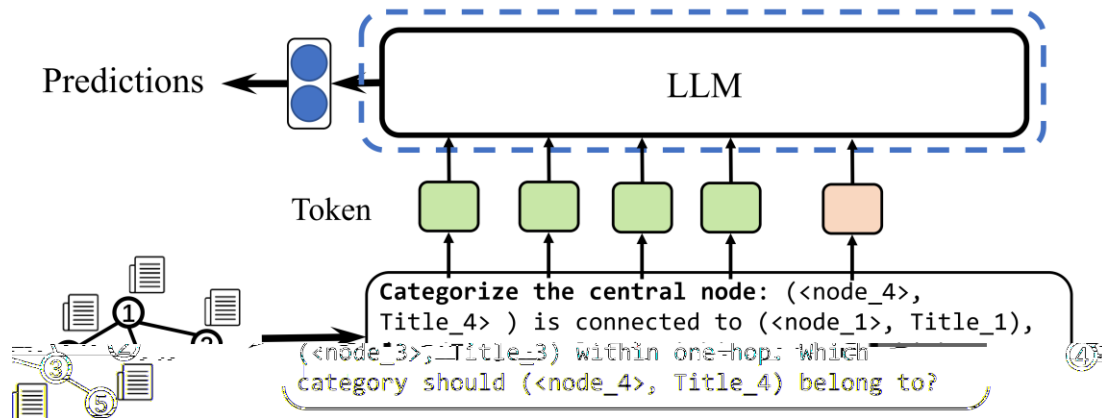
Backbone Architectures

□ Graph-to-Token

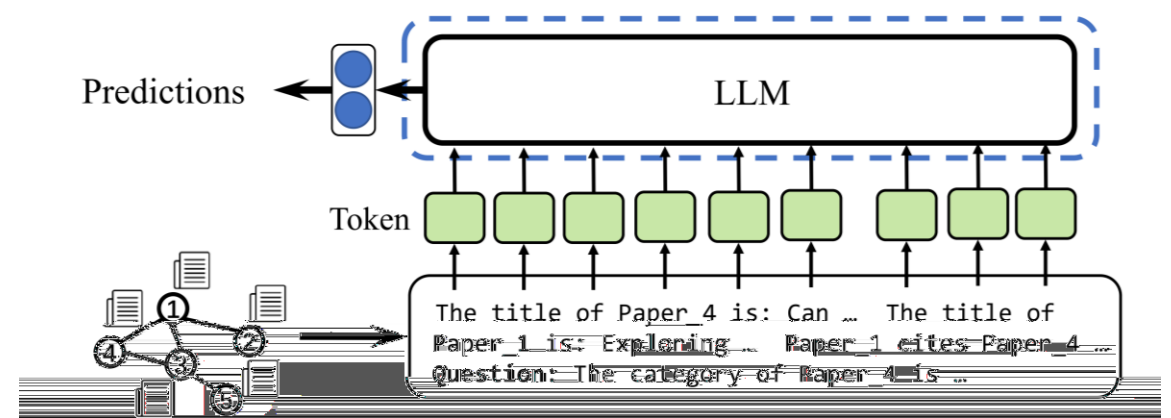
- Tokenize graph information to align it with LLM

□ Graph-to-text

- Describe graph information using natural language



(a) Graph-to-token.



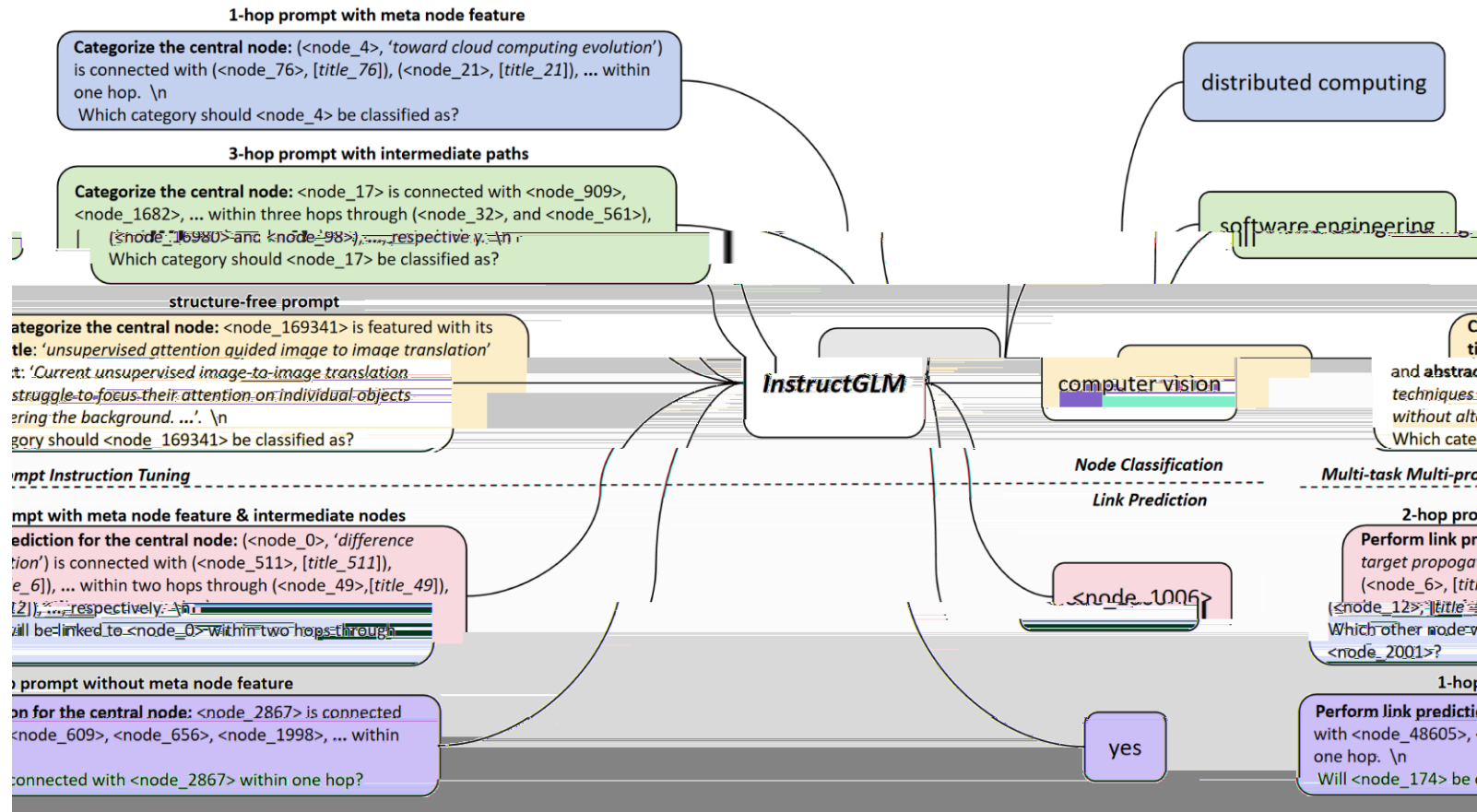
(b) Graph-to-text.

Graph-to-Token: GIMLET

- ❑ Integrating graph data with textual data
- ❑

Graph-to-Token: InstructGLM

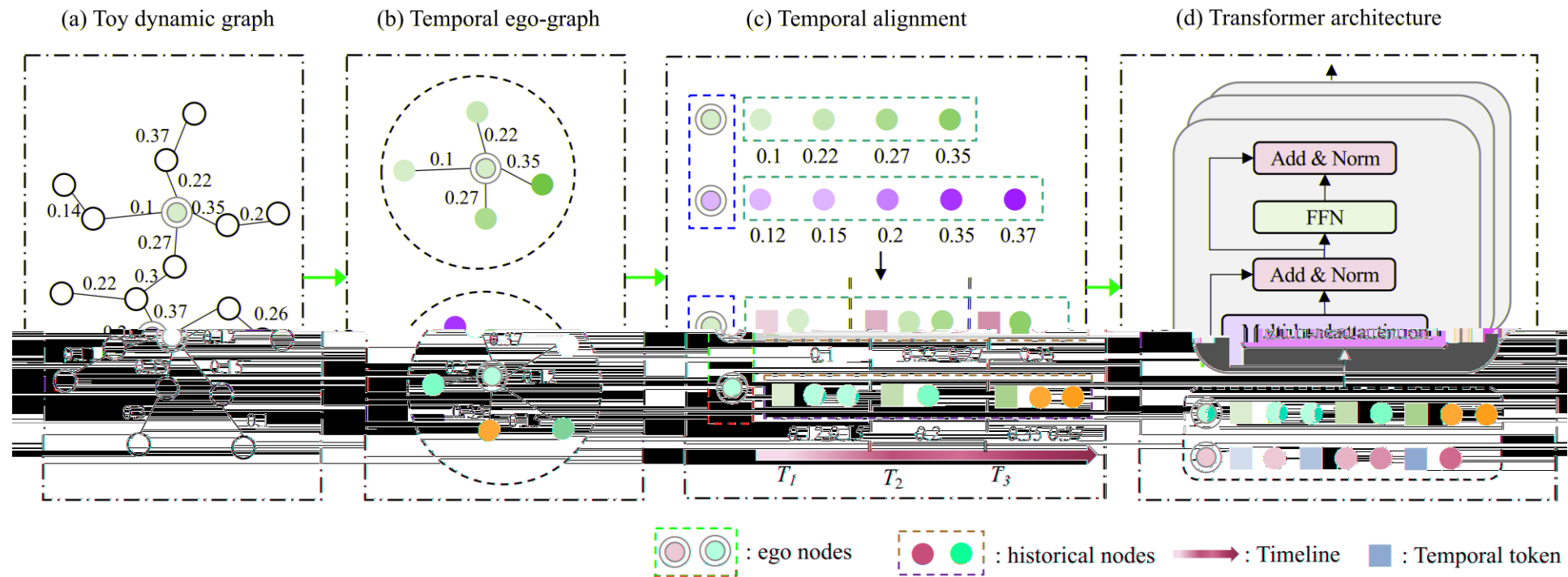
- Expand the vocabulary of the LLM by graph node features



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

Graph-to-Token: SimpleDyG

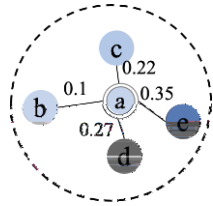
- ❑ Transformer-based approach for dynamic graphs
- ❑ Map a dynamic graph into a set of sequences



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:

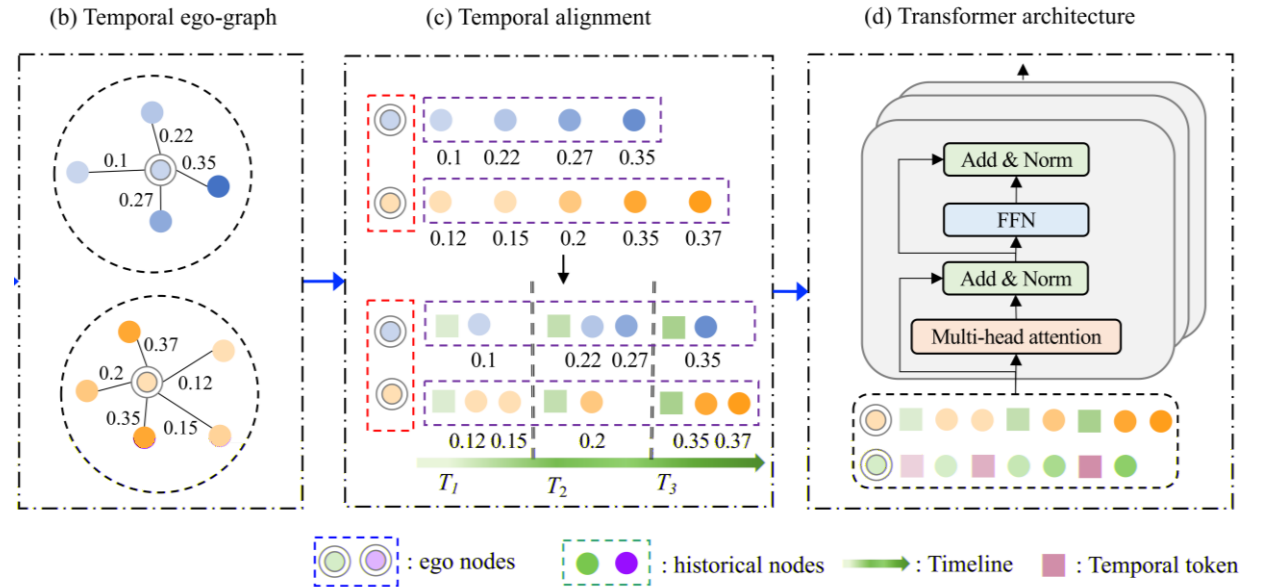
- Segment the time domain:

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

- Sequence for Transformer:

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

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



Graph-to-text

Describe graph information for various graphs and tasks

1. Connectivity
Determine if there is a path between two nodes in the graph. Note that (i, j) means that node i and node j are connected with an undirected edge. Graph: $(0,1) (1,2) (3,4) (4,5)$
Q: Is there a path between node 1 and node 4?

2. Cycle
In an undirected graph, (i, j) means that node i and node j are connected with an undirected edge. The nodes are numbered from 0 to 5, and the edges are: $(3,4) (3,5) (1,0) (2,5) (2,0)$
Q: Is there a cycle in this graph?

3. Topological Sort
In a directed graph with 5 nodes numbered from 0 to 4: node 0 should be visited before node 4, ...
Q: Can all the nodes be visited? Give the solution.

4. Shortest Path
In an undirected graph, the nodes are numbered from 0 to 4, and the edges are: an edge between node 0 and node 1 with weight 2, ...
Q: Give the shortest path from node 0 to node 4.

5. Maximum Flow
In a directed graph, the nodes are numbered from 0 to 3, and the edges are:
an edge from node 0 to node 1 with capacity 10,
an edge from node 0 to node 2 with capacity 6,
an edge from node 2 to node 3 with capacity 4.
Q: What is the maximum flow from node 0 to node 3?

6. Bipartite Graph Matching
job applicants: 0, 1, 2, 3
jobs: 0, 1, 2, 3, 4
There are 4 job applicants numbered from 0 to 3, and 5 jobs numbered from 0 to 4. Each applicant is interested in:
Applicant 0 is interested in jobs 1, 2, 3, 4.
Q: Find an assignment of jobs to applicants in such that the maximum number of applicants find the job they are interested in.

7. Hamilton Path
In an undirected graph, (i, j) means that node i and node j are connected with an undirected edge. The nodes are numbered from 0 to 4, and the edges are: $(4,2) (0,2) (4,3) (0,1) (0,2) (4,1) (2,3)$.
Q: Is there a path in this graph that visits every node exactly once? If yes, give the path. Note that in a path, adjacent nodes must be connected with edges.

8. GNN
In an undirected graph, the nodes are numbered from 0 to 4, and every node has an embedding. (i, j) means that node i and node j are connected with an undirected edge. Embeddings: node 0: $(1, 1)$, node 1: $(0, 2)$, node 2: $(4, 1)$, node 3: $(0, 1)$, node 4: $(0, 1)$.
In a simple graph convolution layer, each node's embedding is updated by the sum of its neighbors' embeddings.
Q: What is the embedding of each node on the next layer of samples?

Graph description language

Graph Structured Data
Knowledge Graph, Collaboration Network, Molecular Graph

Graph description language:

```
<?xml version='1.0' encoding='utf-8'?>
<graphml xmlns="http://graphml.graphdrawing.org/xmlns">
  <key id="relation" for="edge" attr.name="relation" attr.type="string" />
  <key id="title" for="node" attr.name="title" attr.type="string" />
  <graph edgedefault="undirected">
    <node id="P357">
      <data key="title">statistical anomaly detection via composite hypothesis models</data>
    </node>
    <node id="P79639">
      <data key="title">universal and composite hypothesis testing</data>
    </node>
    <edge source="P357" target="P79639">
      <data key="relation">reference</data>
    </edge>
  </graph>
</graphml>
```

Graph-Syntax Tree

Graph-Syntax Tree

label: 1st-hop: [A] 2nd-hop: [B]
feature: center-node: [0] 1st-hop: [1, 2] 2nd-hop: [3, 2]

Text Attributes
feature x (green square)
label y (blue square)

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 Architectures

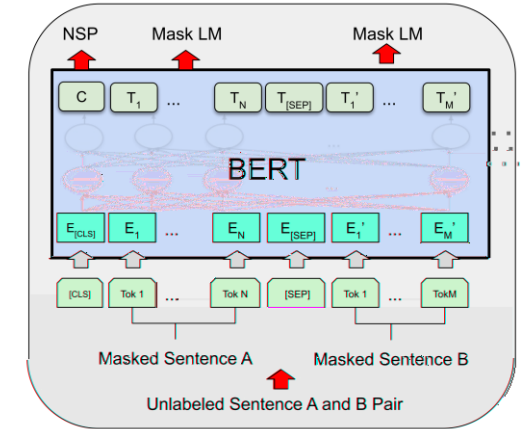
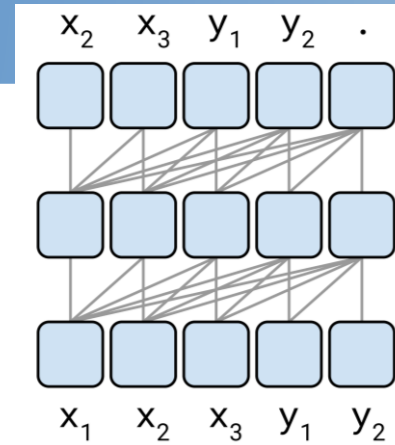
□ Pre-training

□ Adaptation

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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

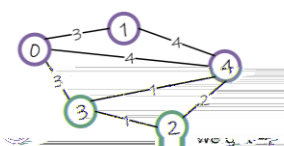
- Backbone Architectures
- Pre-training
- **Adaptation**

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Table 3. Details of approaches involved as LLM based models

Adaptation

Standard Prompting



graph>
graph, the nodes are
0 to 4, and the edges are
node 0 and node 4 with
weight 4.

Let's construct a graph with the nodes and edges first.

Q: Give the shortest path from node 0 to node 2.

A: All the paths from node 0 to node 2 are:
0,3,2 with a total weight of $3 + 1 = 4$,
0,1,4,2 with a total weight of $3 + 4 + 2 = 9$,
0,4,3,2 with a total weight of $4 + 1 + 1 = 6$.
The weight of path 0,3,2 is the smallest, so the shortest path from node 0 to node 2 is 0,3,2 with a total weight of 4.

Build-a-Graph Prompting

<in-context exemplar>
In an undirected graph, the nodes are numbered from 0 to 4, and the edges are: an edge between node 0 and node 4 with weight 4.

Let's construct a graph with the nodes and edges first.

Q: Give the shortest path from node 0 to node 2.

A: All the paths from node 0 to node 2 are:
0,3,2 with a total weight of $3 + 1 = 4$,
0,1,4,2 with a total weight of $3 + 4 + 2 = 9$,
0,4,3,2 with a total weight of $4 + 1 + 1 = 6$.
The weight of path 0,3,2 is the smallest, so the shortest path from node 0 to node 2 is 0,3,2 with a total weight of 4.

Algorithmic Prompting

We can use a Depth-First Search (DFS) algorithm to find the shortest path between two given nodes in an undirected graph. The basic idea is to start at one of the nodes and use DFS to explore all of its adjacent nodes. At each node you can keep track of the distance it takes to reach that node from the starting node. Once you have explored all the adjacent nodes you can backtrack and pick the node which has the shortest distance to reach the destination node.

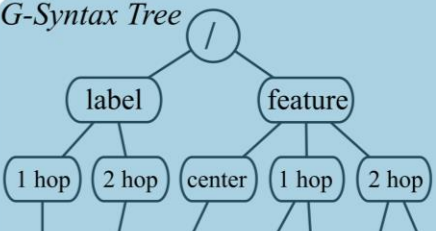
<in-context exemplar>
In an undirected graph, the nodes are numbered from 0 to 4 and the edges are: an edge between node 0 and node 4 with weight 4, an edge between node 0 and node 3 with weight 3, an edge between node 0 and node 1 with weight 3, an edge between node 1 and node 4 with weight 4, an edge between node 3 and node 2 with weight 1, and an edge between node 4 and node 2 with weight 2.

Q: Give the shortest path from node 0 to node 2.

A: All the paths from node 0 to node 2 are:
0,3,2 with a total weight of $3 + 1 = 4$,
0,1,4,2 with a total weight of $3 + 4 + 2 = 9$,
0,4,3,2 with a total weight of $4 + 1 + 1 = 6$.
The weight of path 0,3,2 is the smallest, so the shortest path from node 0 to node 2 is 0,3,2 with a total weight of 4.

(c) GraphText

G-Syntax Tree

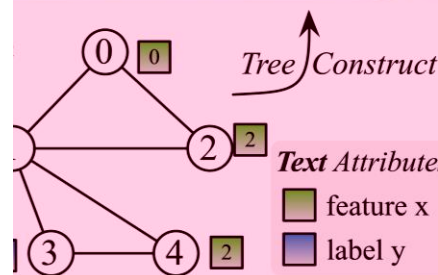


→ Traverse →

Task prompt and demos

Graph information:
label: G-Prompt
1st-hop: [A]
2nd-hop: [B]
feature:
center-node: [0]
1st-hop: [1, 2]
2nd-hop: [3, 2]

Tree Construct



Text Attributes
■ feature x
■ label y

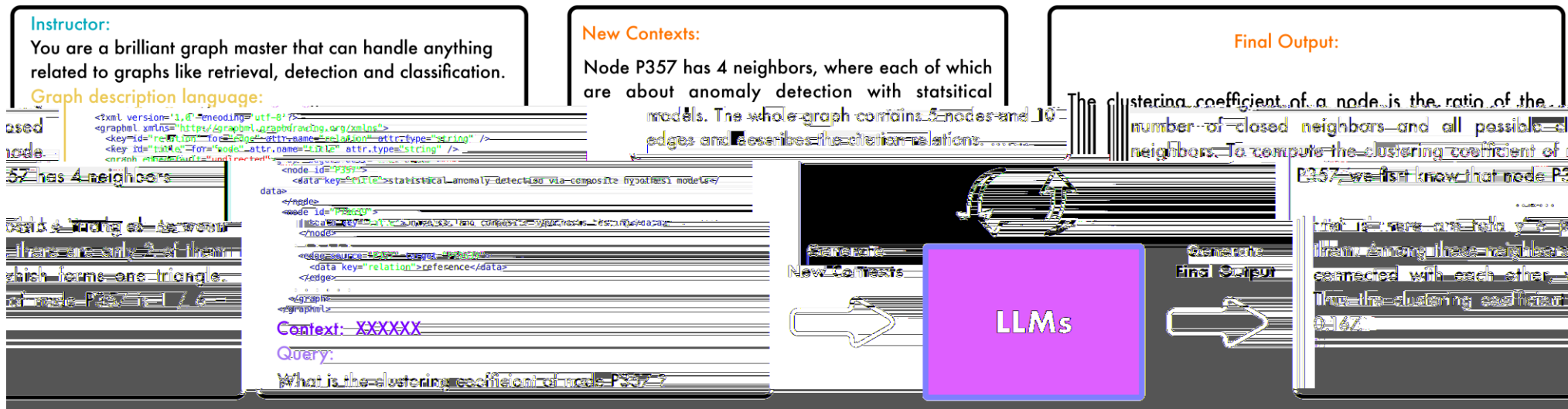
Question: What's the category of the node (choose from [A, B])?

According to the demos, 1st-hop labels are robust predictions. Therefore, the answer is A.

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 Architectures

□ 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
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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

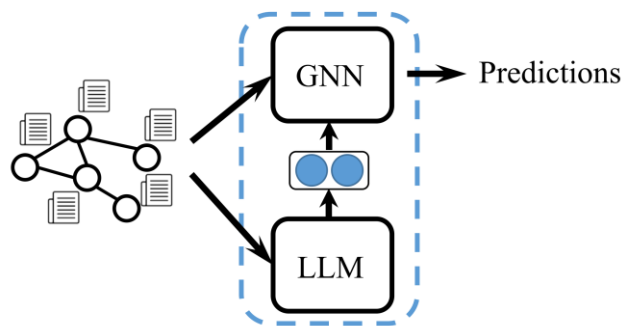
- LLMs extract node features from raw data; GNNs make predictions

□ Symmetric Methods

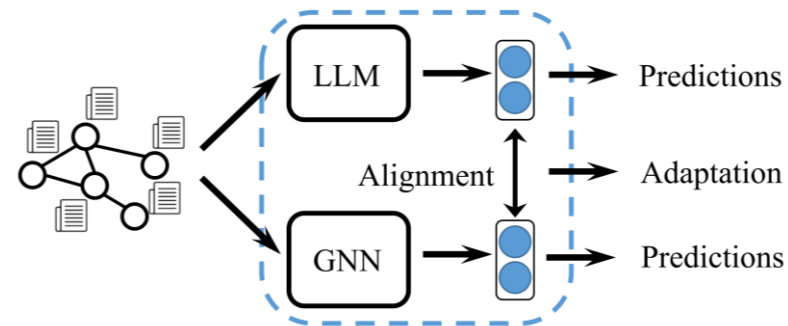
- Align the embeddings of GNN and LLM

□ LLM-centric Methods

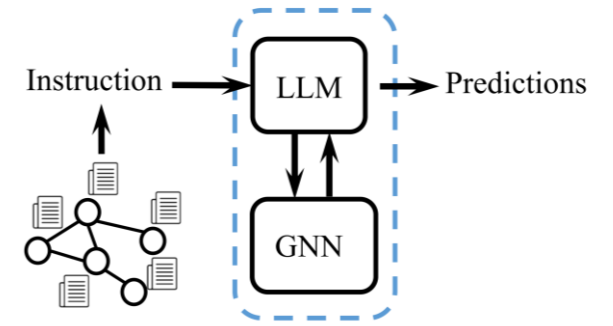
- Utilize GNNs to enhance the performance of LLM



(a) GNN-centric methods.



(b) Symmetric methods.

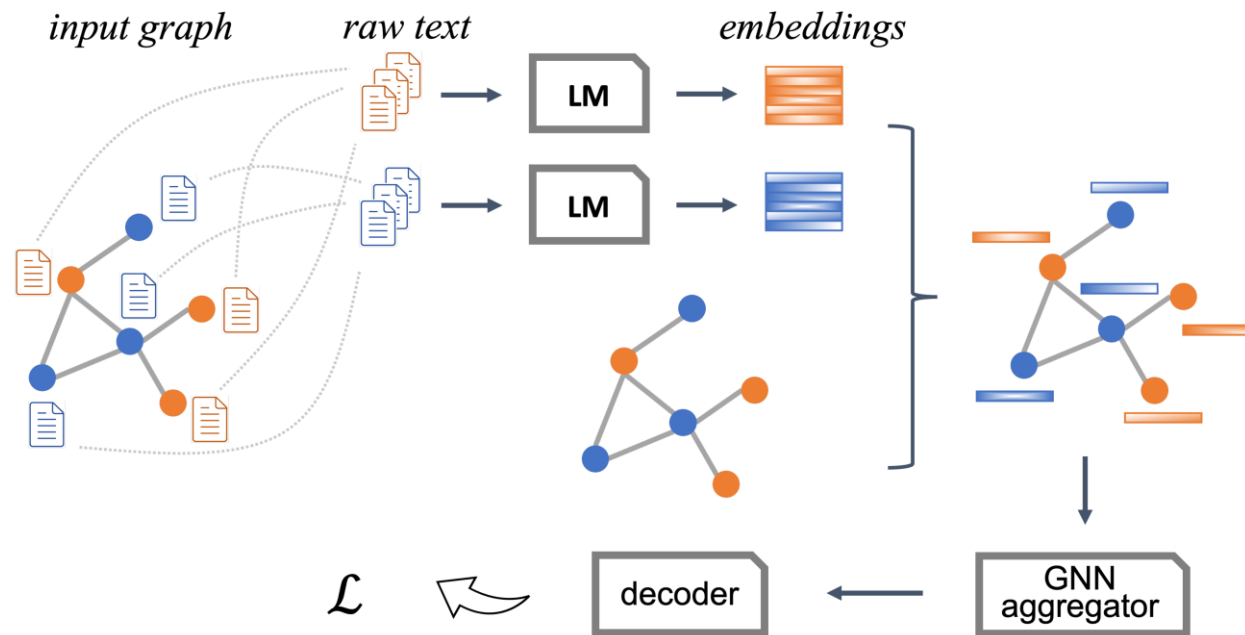


(c) LLM-centric methods.

GNN-centric Methods: GaLM

□ The backbone model:

Raw text \rightarrow LMs \rightarrow GNN aggregator \rightarrow decoder



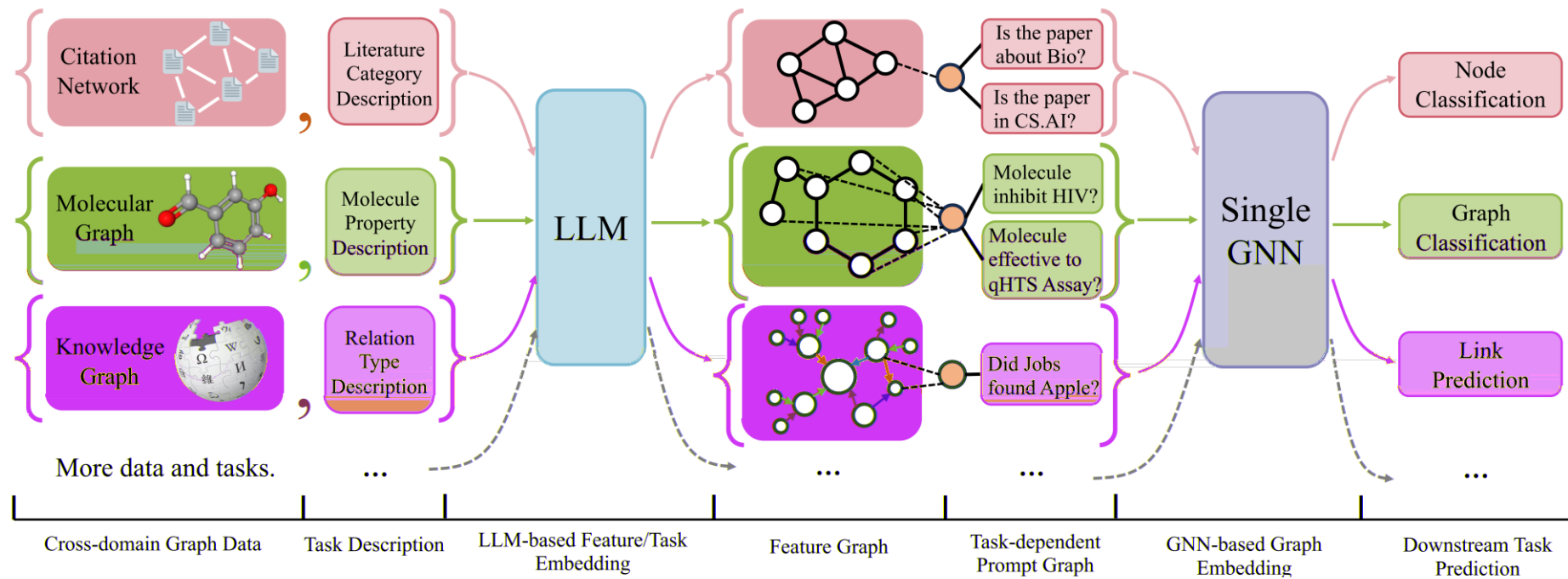
Xie, et al. "Graph-aware language model pre-training on a large graph corpus can help multiple graph applications."

GNN-centric Methods: One for all

□ The backbone model:

Text-attributed graph
Task description

LLMs → Prompted graph → GNN → Downstream tasks

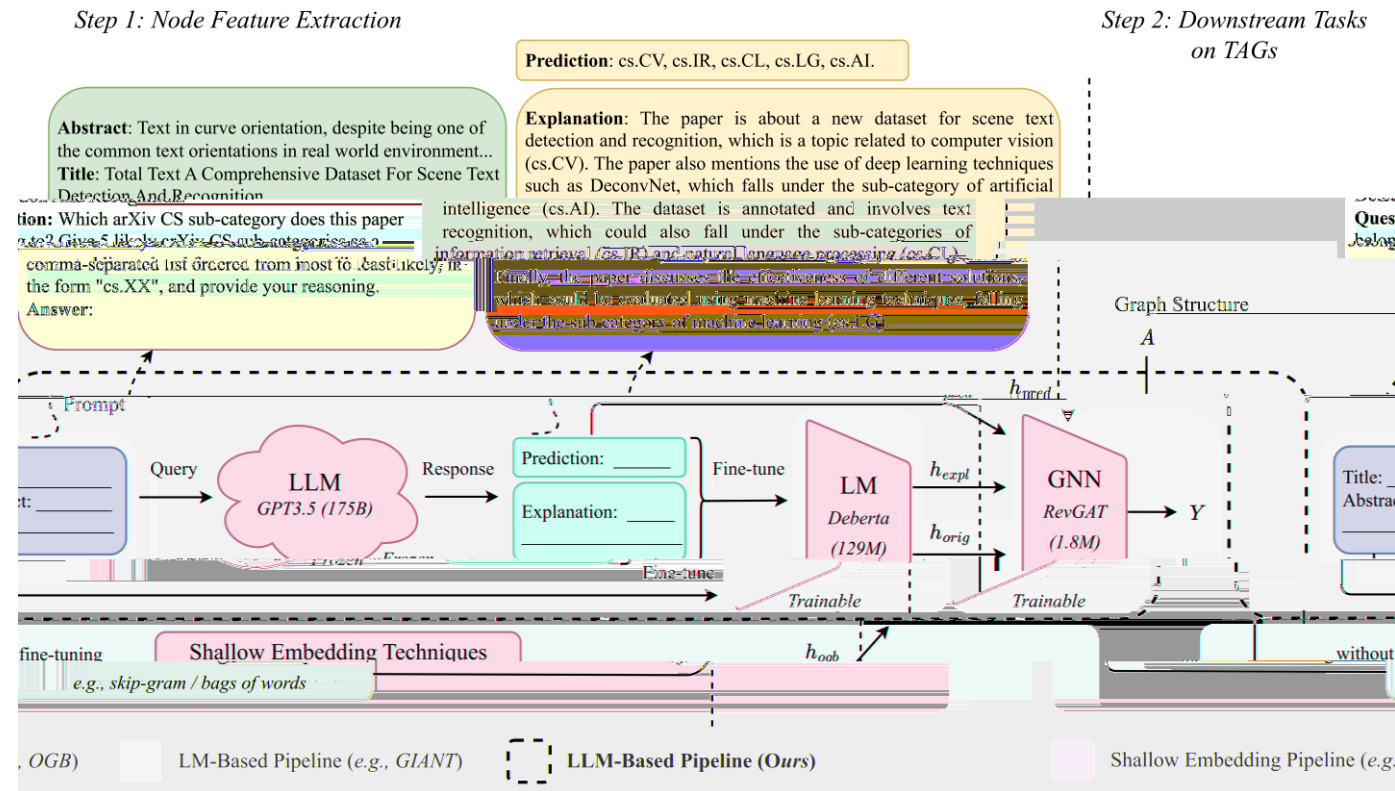


Liu, et al. "One for all: Towards training one graph model for all classification tasks."

GNN-centric Methods: TAPE

□ The backbone model:

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

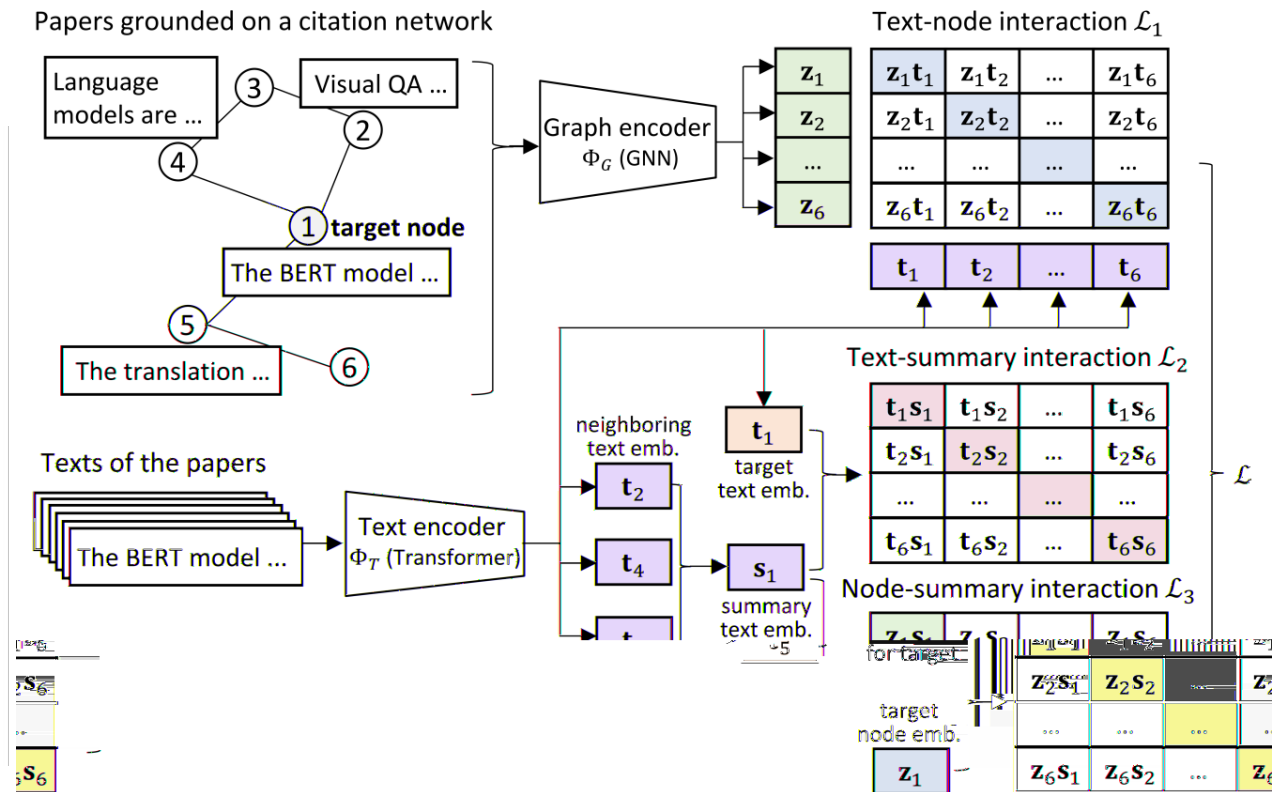
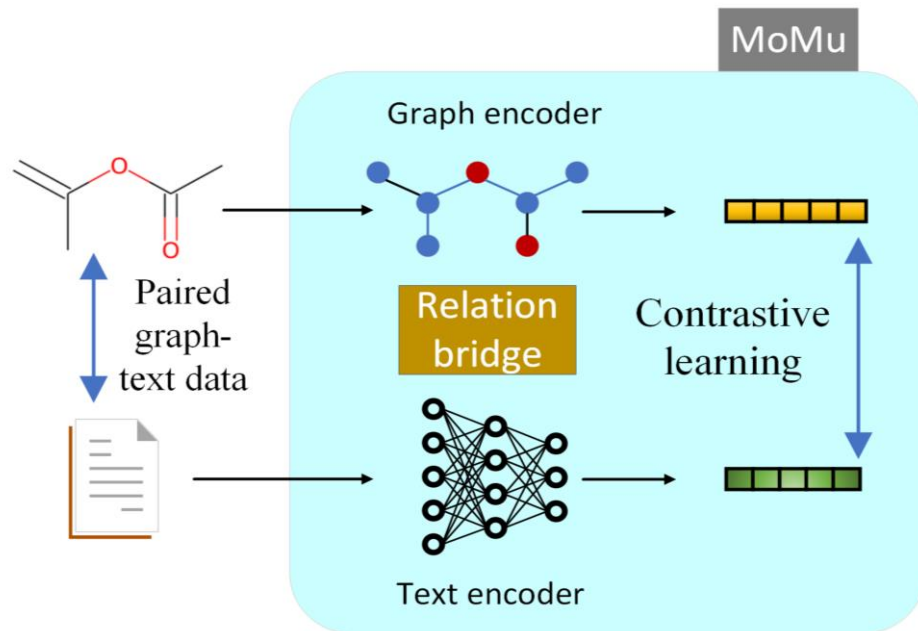


He, et al. "Harnessing explanations: LLM-to-LM interpreter for enhanced text-attributed graph representation learning."

Symmetric Methods: MoMu, G2P2

□ The backbone model:

- Dual encoders: Graph & Text encoder
- Contrastive Learning



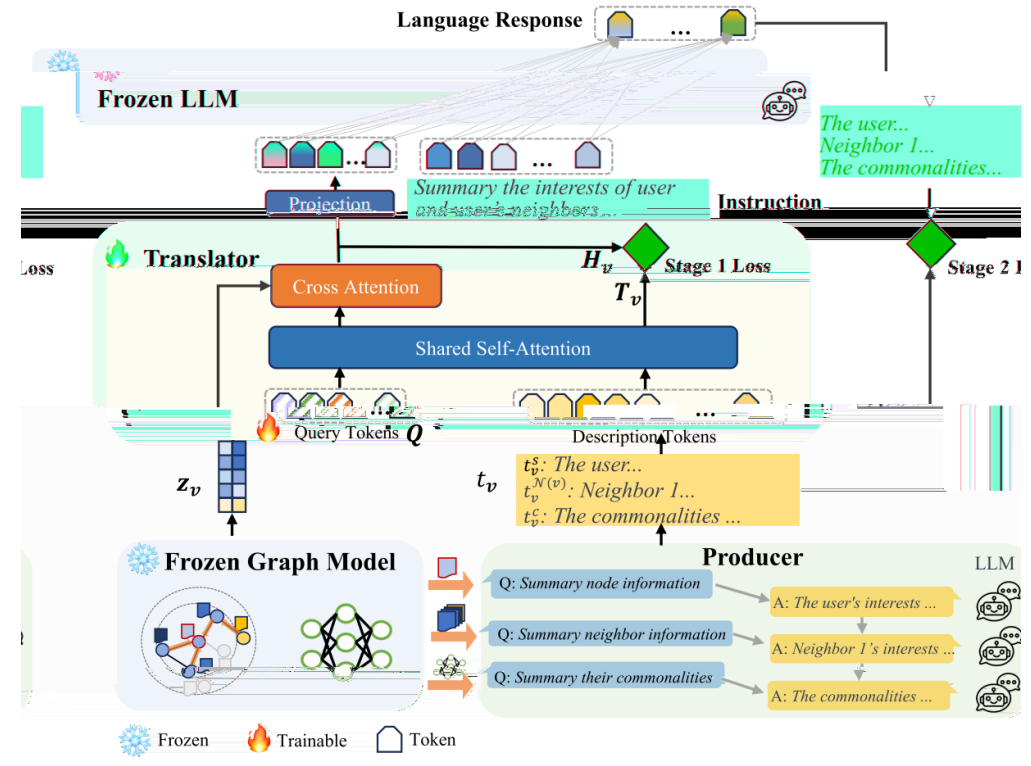
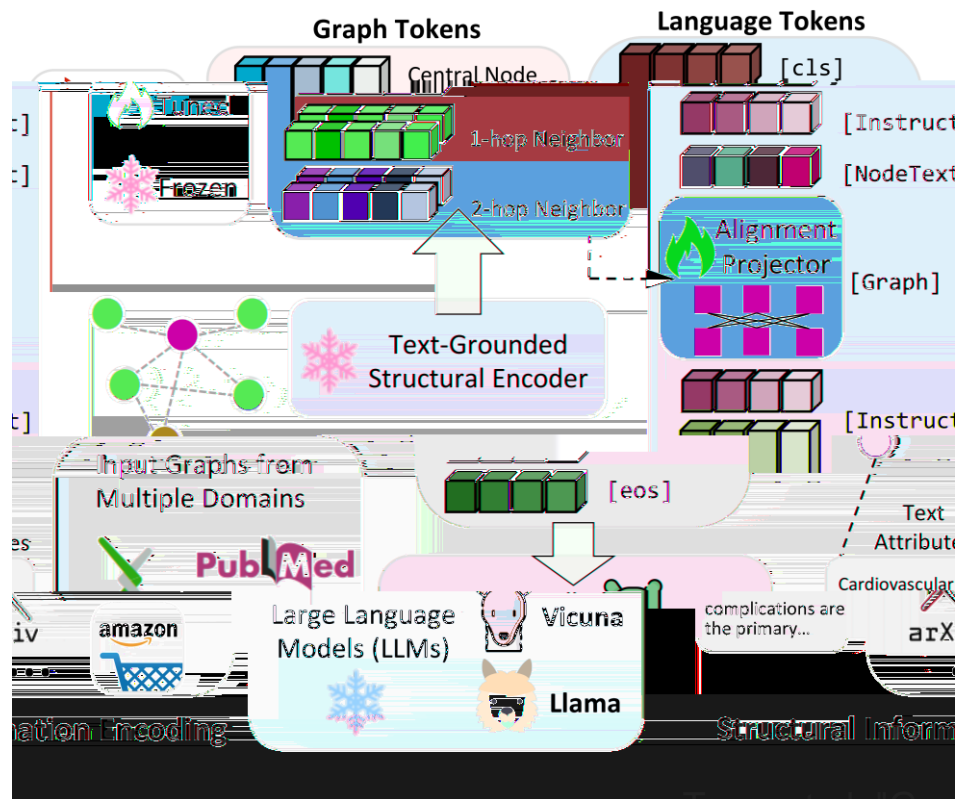
Su, et al. "A molecular multimodal foundation model associating molecule graphs with natural language."

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

LLM-centric Methods: GraphGPT, GraphTranslator

□ The backbone model:

Graph \rightarrow GNN \rightarrow Projection \rightarrow LLM



Yang, 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 Architectures

□ Pre-training

□ Adaptation

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Pre-training

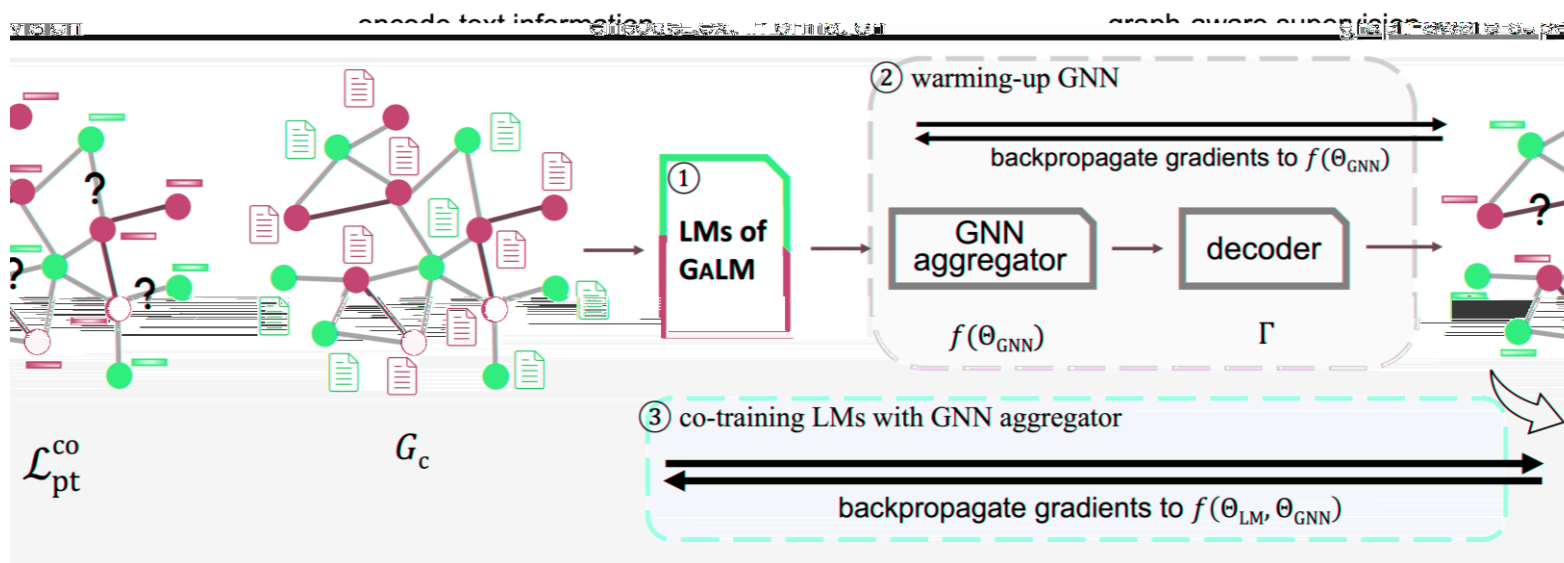
□ GNN or LLM-based

- Masked Language Modeling
- Language Modeling
- Text-Text Contrastive Learning
- Graph reconstruction

□ Alignment-based

- Graph-Text Contrastive Learning

GNN or LLM-based: GaLM

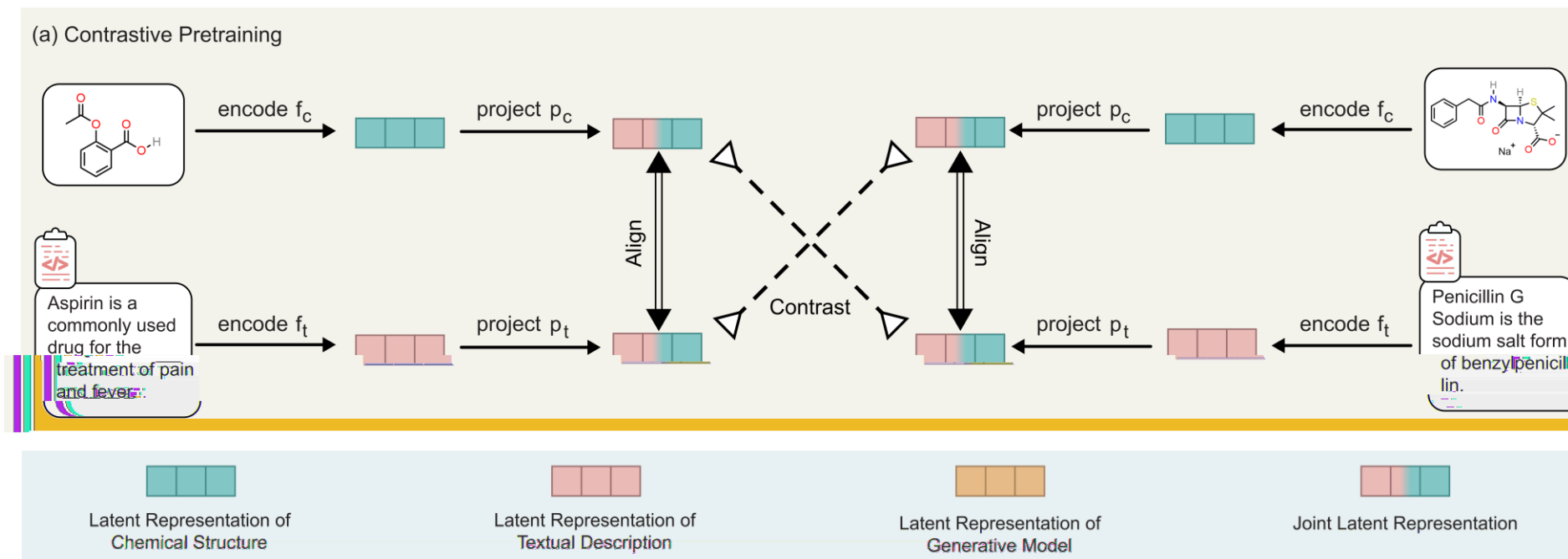


Xie, et al. "Graph-aware language model pre-training on a large graph corpus can help multiple graph applications."

Alignment-based: MoleculeSTM

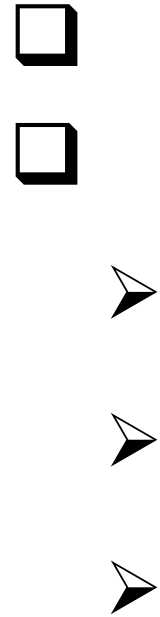
□ Graph-Text Contrastive Learning (GTCL)

- Map the graph and text representations extracted to a joint space using two projectors (p_c and p_t) via contrastive learning

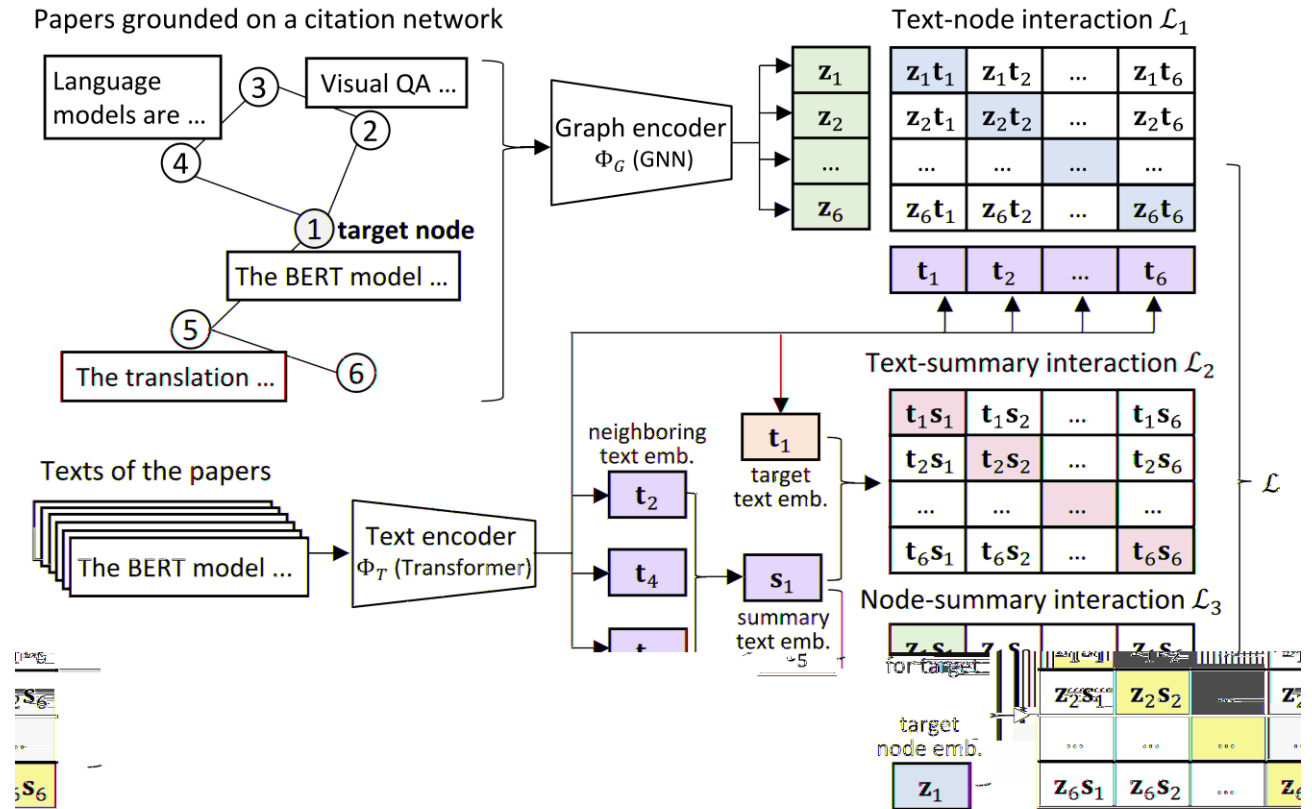


Liu, et al. "Multi-modal molecule structure–text model for text-based retrieval and editing." *Nature Machine Intelligence* 2023

Alignment-based: G2P2



$$s_i = \frac{1}{L} \sum_{j=1}^L t_j$$



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

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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

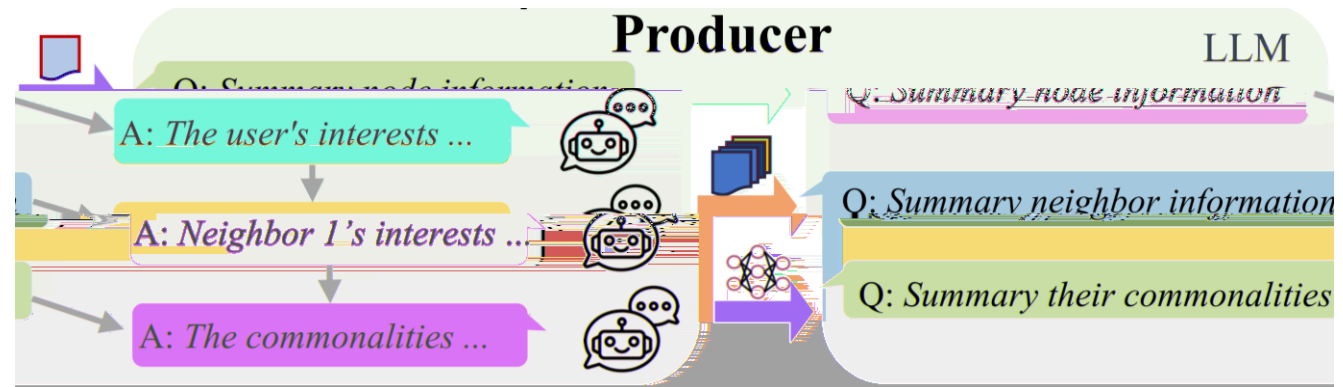
PEFT: GraphTranslator

□ Producer:



CoT) ->LLM->high-quality description

- node information
- neighbor information
- commonalities



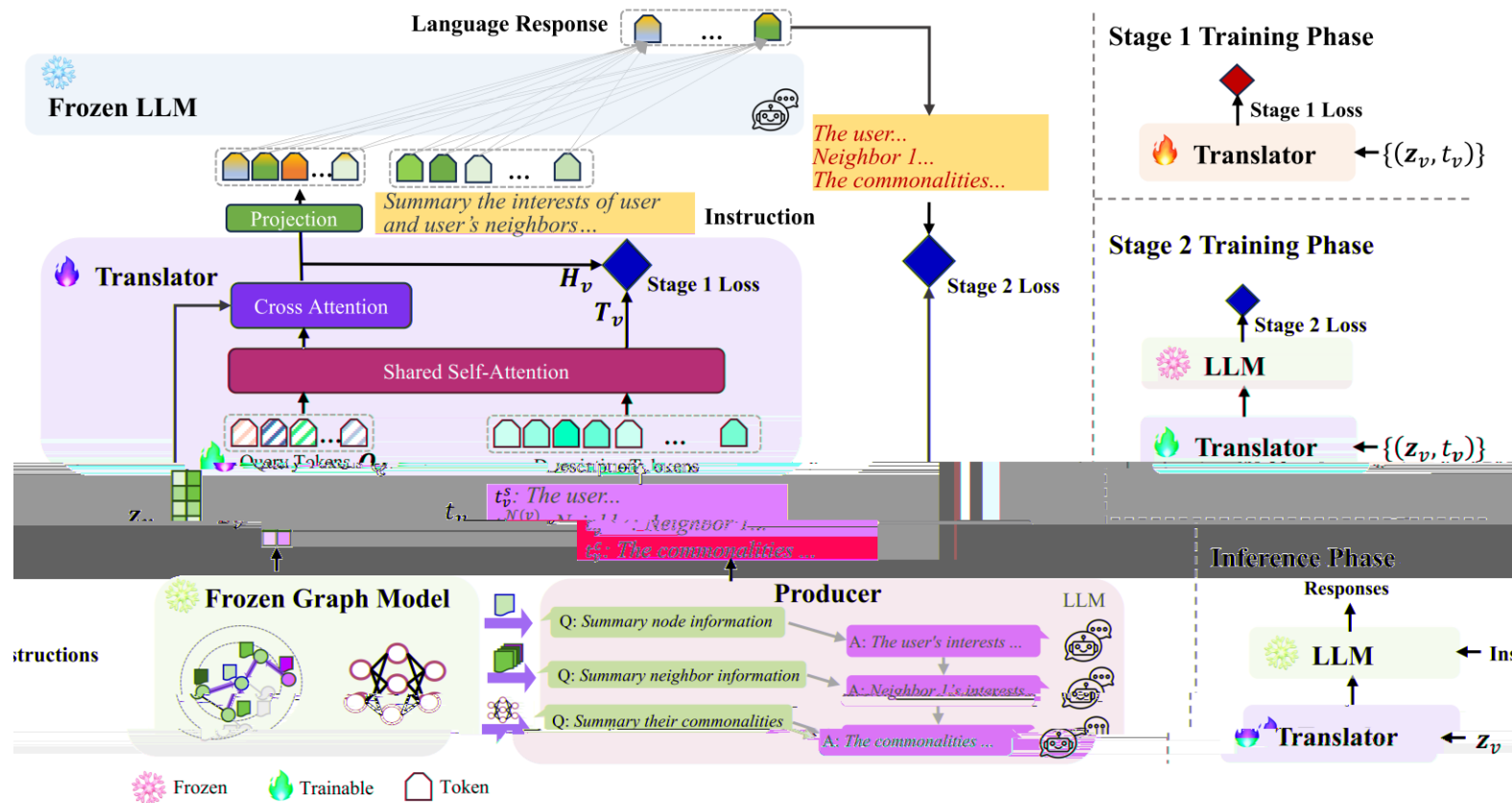
□ Prompt template:

Dataset	Step	Prompt
Taobao	User behavior summary	User Behavior Description: <i><User Behavior Description></i> . 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: <i><Neighbor Behavior Description></i> . 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



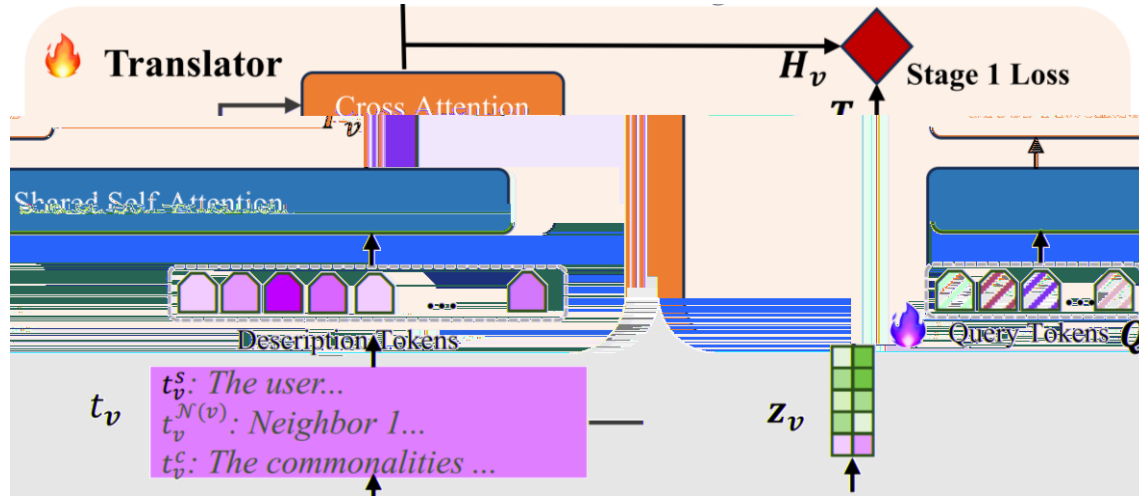
➤ Stage 1: Align graph-text

➤ Stage 2: Align graph-LLM

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PEFT: GraphTranslator

□ Training: Stage 1

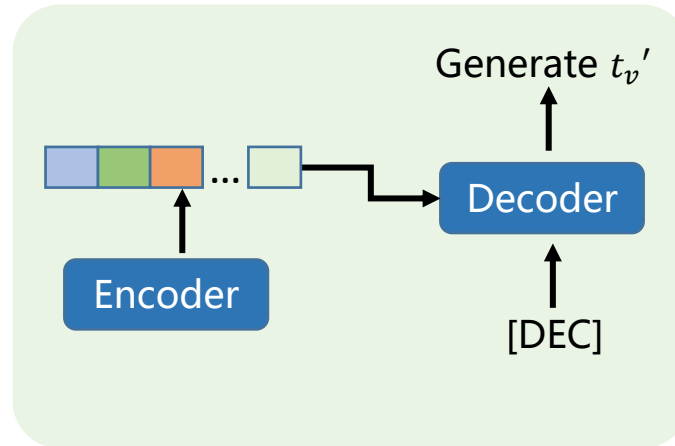


$$H_v = \{h_{v,i}\}_{i=1}^M$$

Node Representation

$$T_v = \{\tilde{t}_{v,i}\}_{i=1}^L$$

Text Representation

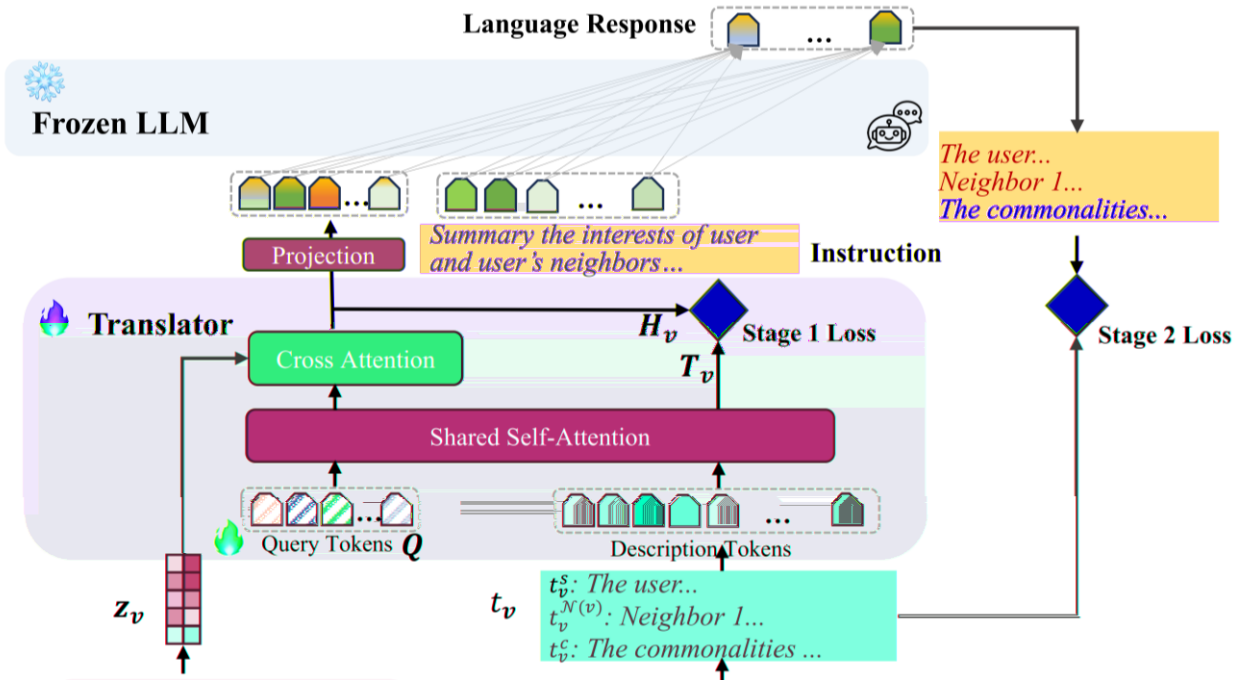


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PEFT: GraphTranslator

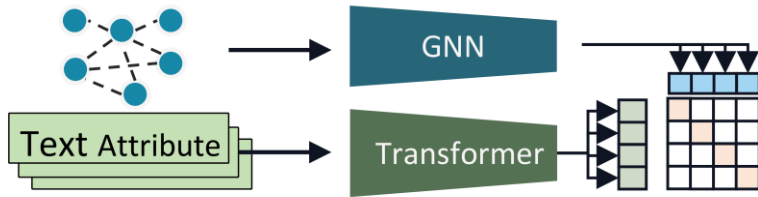
□ Training: Stage 2



- 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
 - Align the response text of LLM with the actual descriptive text

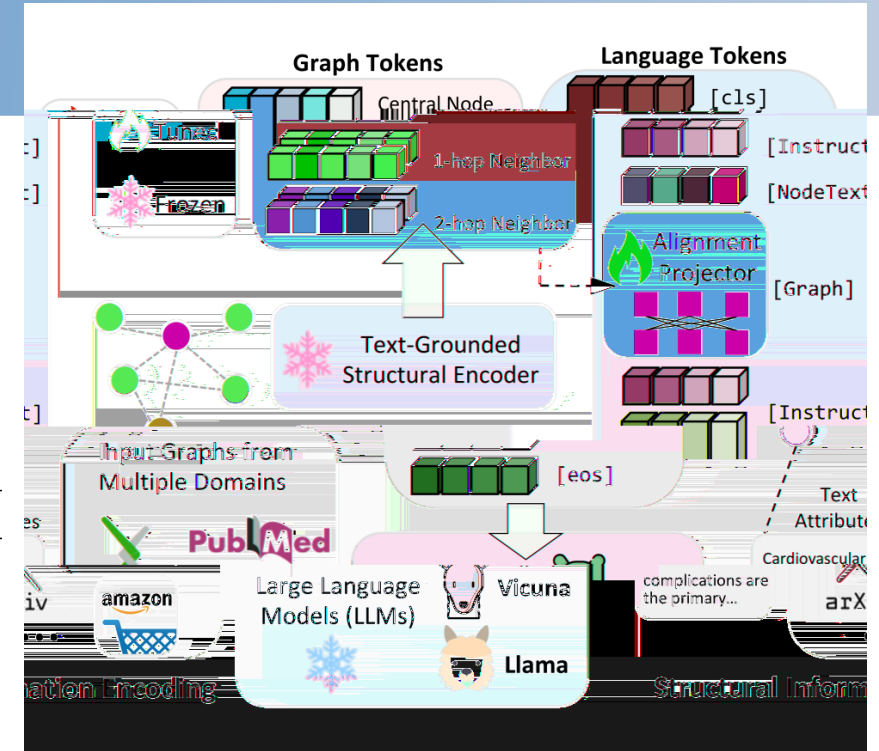
PEFT: GraphGPT

□ Graph: Text-Grounded Structural Encoder



□ Projector: Map graph representation to LLM

□ Instruction Tuning: Only fine-tune projector

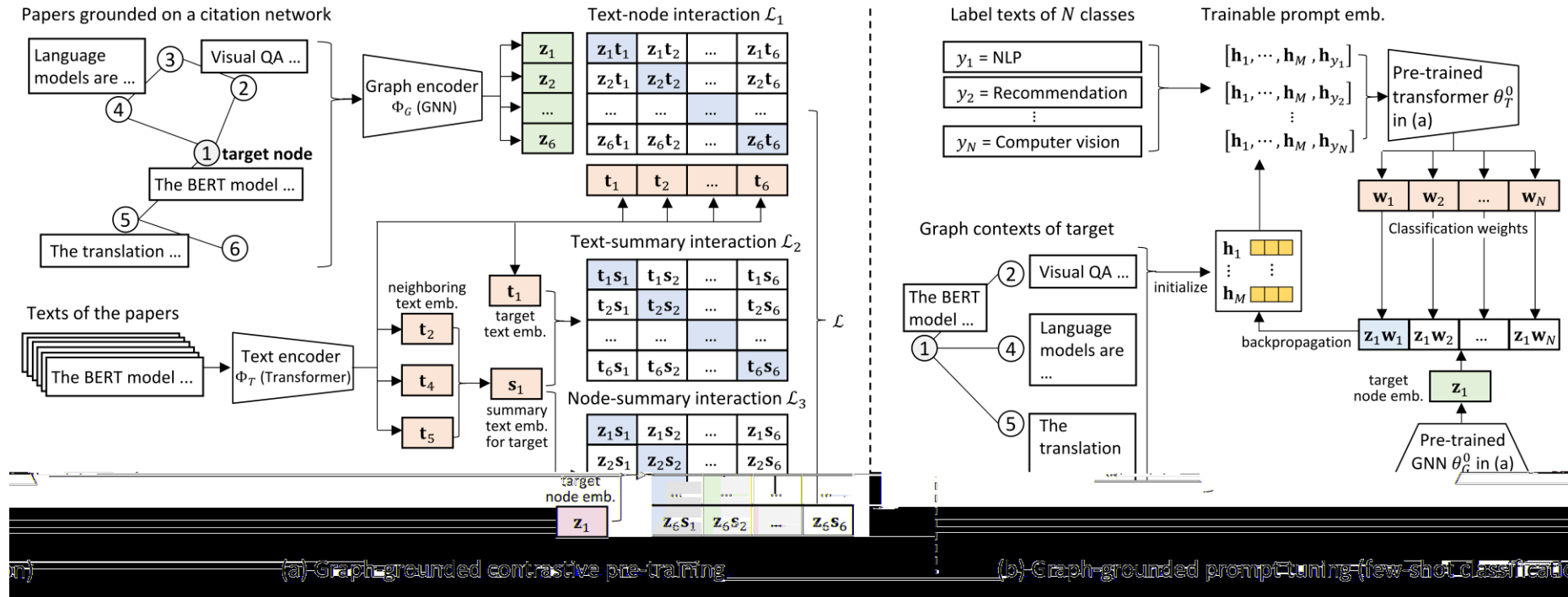


```
Graph Information: <graph>: Central Node: 68442, Edge index: [[...src node...],[...dst node...]], Node list: [...]  
Human Question: Given a sequence of graph tokens: <graph> that constitute a subgraph of a citation graph, ...  
2: ..., please reorder the list of papers according to the order of graph tokens:  
1  
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  
Node Classification: Graph Information: <graph>: Central Node: 2, Edge index: [[...src node...],[...dst node...]], Node list: [...]  
Information: Abstract: ... Title: ...  
is likely to belong to cs.IT...  
Link Prediction  
Graph Information: <graph>: Central Node 1: 8471, Edge index 1: [[...src node...],[...dst node...]], Node list 1: [...]  
<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, ...  
sequence of graph tokens: <graph>, ... Abstract: ... Title: ..., are these two central nodes connected? Give me an  
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."

Prompt-Tuning: G2P2

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

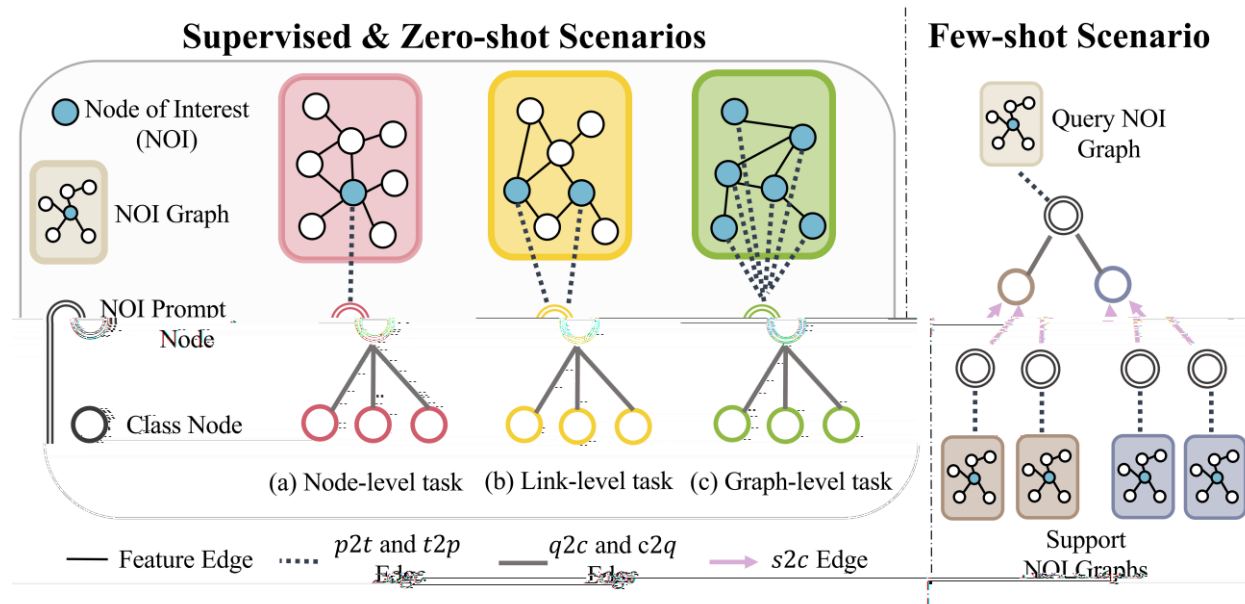


Wen, et al. "Augmenting low-resource text classification with graph-grounded pre-training and prompting."

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. \langle task description \rangle .

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. \langle class description \rangle .

Example: Prompt node. Molecule property. The molecule is effective in: ...

Example: Prompt node. Literature Category: cs AI (Artificial Intelligence). Covers all areas of

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

Outline

□ LLM based Models

- Backbone Architectures
- Pre-training
- Adaptation

□ GNN+LLM based Models

- Backbone Architectures
- 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

