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Towards Graph Foundation Models

WWW 2024 Tutorial

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Towards Graph Foundation Models
Part II: GNN-based Methods

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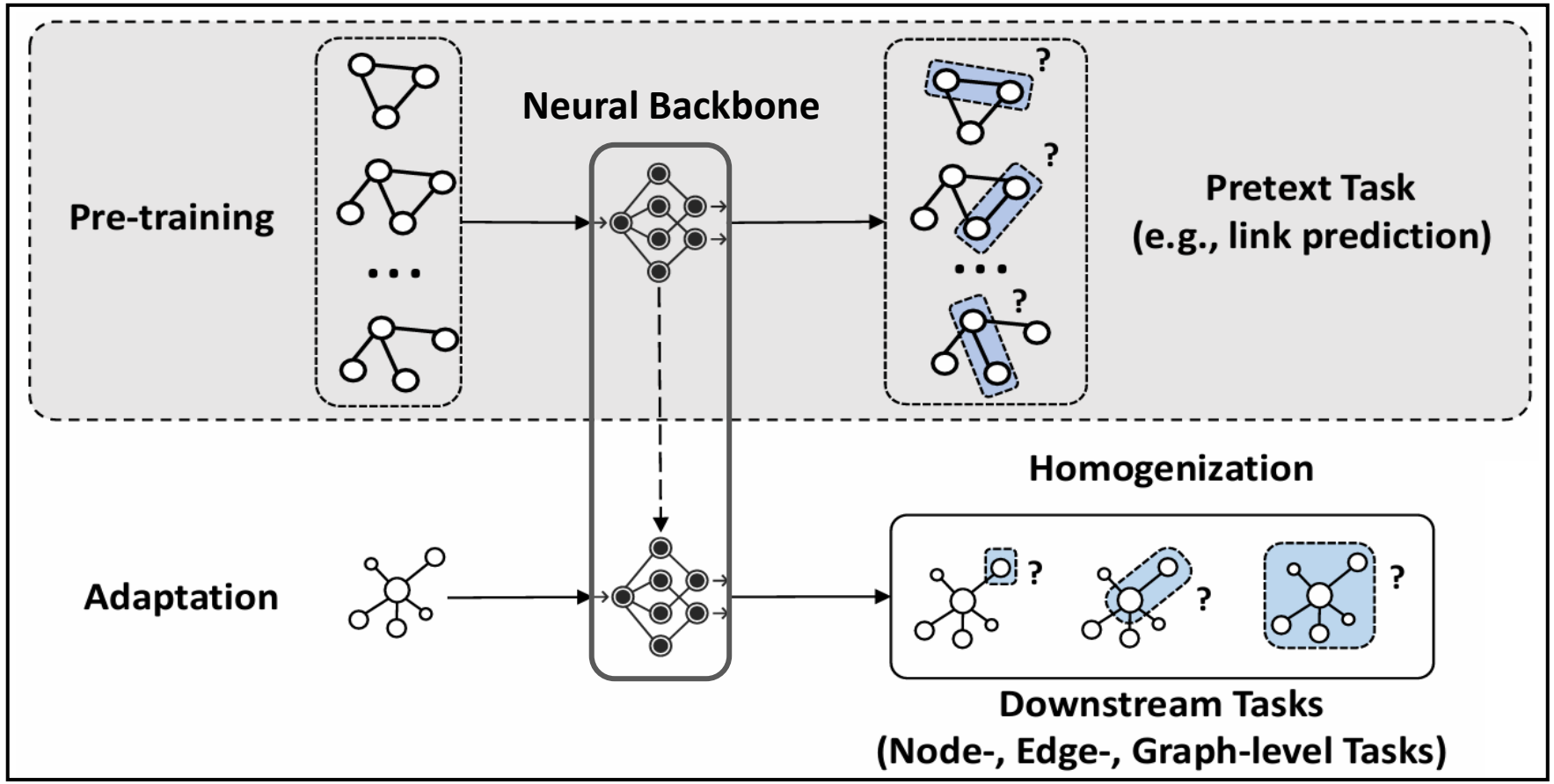
GNN-based Methods

Backbone： No unified architecture

（Message Passing/Graph Transformer）

Paradigm： Pre-training + Adaptation



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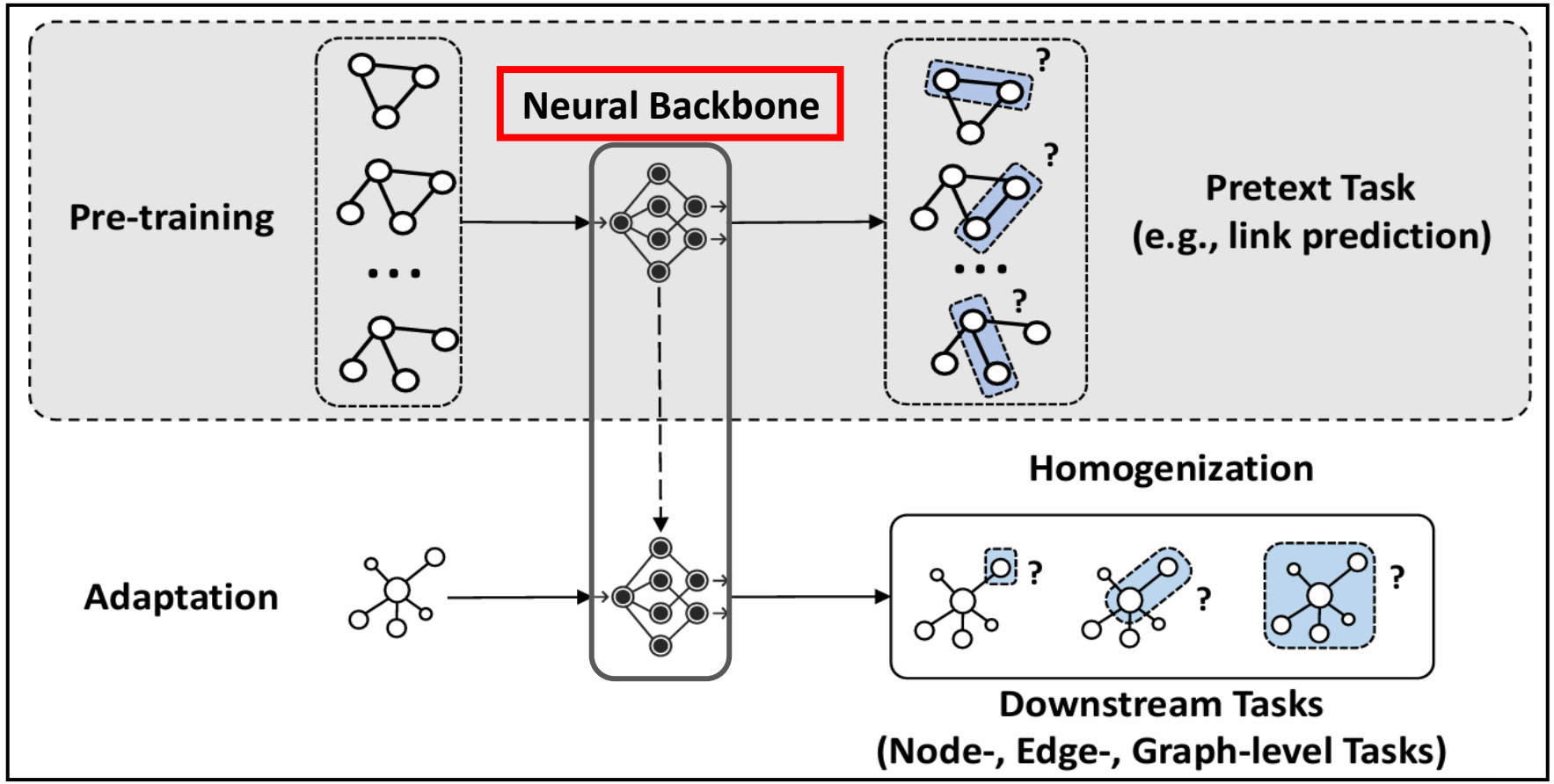

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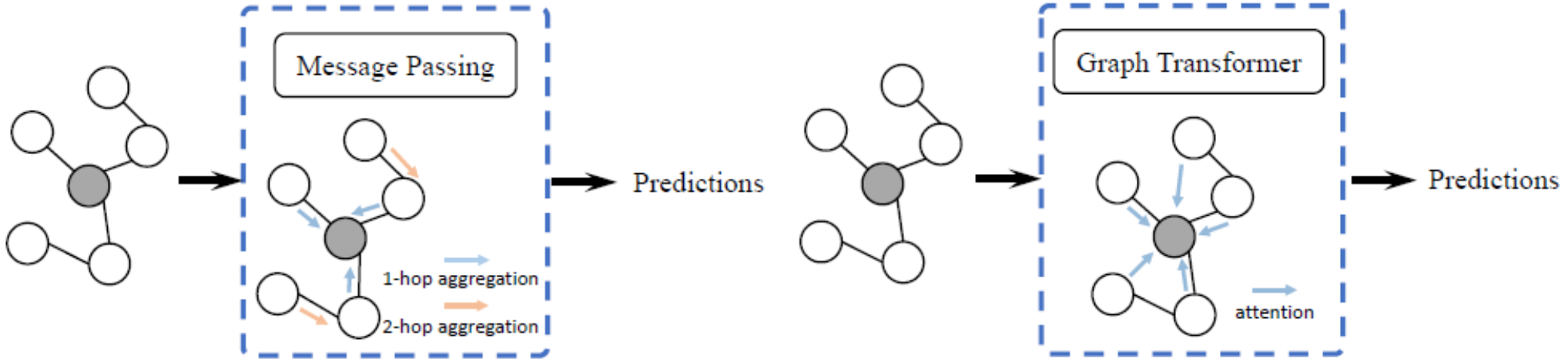
Backbone Architecture

Backbone Architecture

- Message Passing: propagates information between nodes that are explicitly connected in the graph structure
- Graph Transformer: considers and measures the similarity between every pair of nodes in the graph



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

Backbone Architecture

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- Message Passing: propagates information between nodes that are explicitly connected in the graph structure
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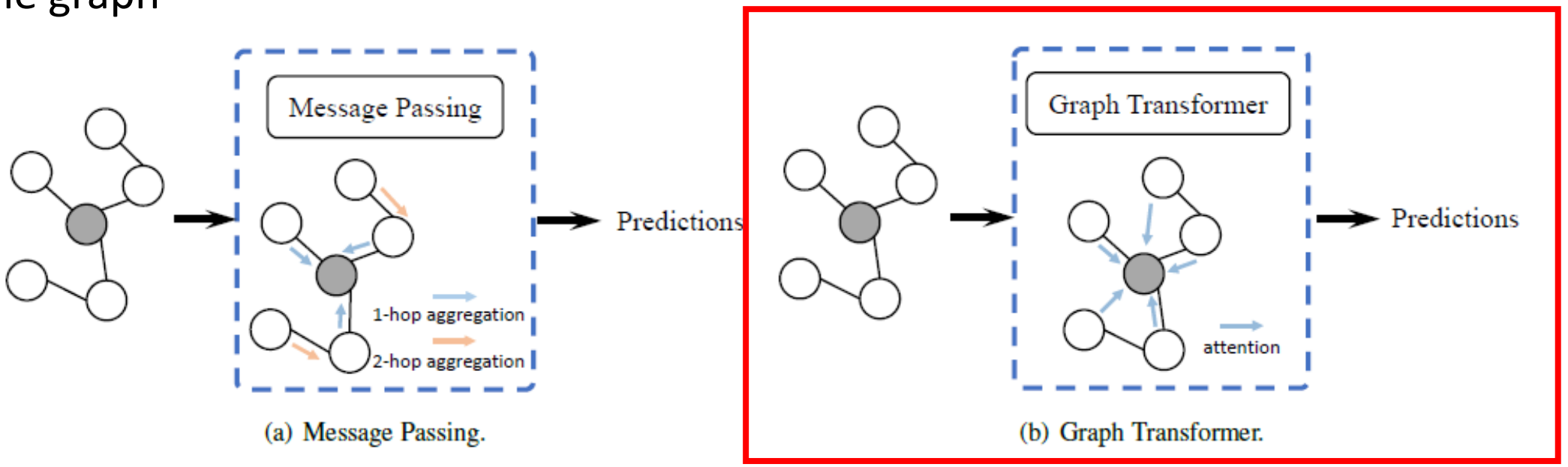


Graphormer

Motivation：

- The Transformer is well acknowledged as the most powerful neural network in modelling sequential data, such as natural language and speech.
- Model variants built upon Transformer have also been shown great performance in computer vision and programming Language.
- However, Transformer has still not been the de-facto standard on public graph representation leaderboards.

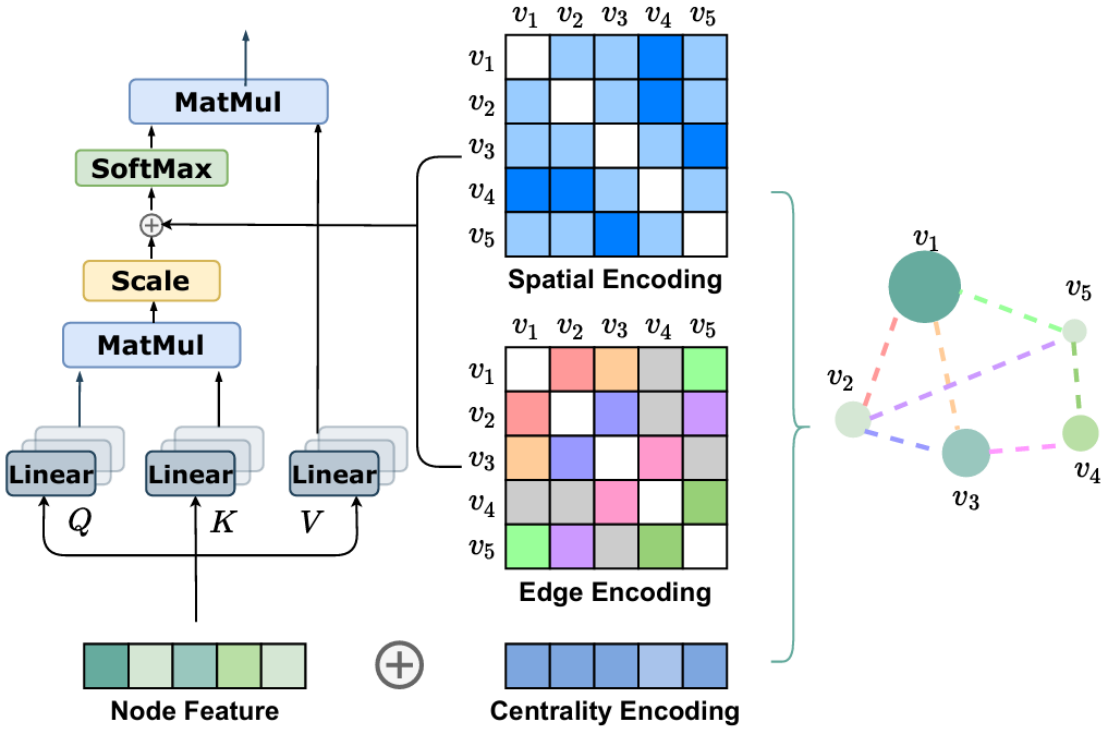
Whether Transformer architecture is suitable to model graphs and how to make it work in graph representation learning?

Chengxuan Ying, Tianle Cai, Shengjie Luo, Shuxin Zheng, Guolin Ke, Di He, Yanming Shen, and Tie-Yan Liu. 2021. Do transformers really perform badly for graph representation? NeurIPS 2021.

Graphormer

Core idea：

- properly incorporate structural information of graphs into the model.
  - propose a Centrality Encoding to capture the node importance in the graph.
  - propose a novel Spatial Encoding to capture the structural relation between nodes
  - design a new Edge Encoding method to take such signal into the Transformer layers.



Graphormer

Structural Encodings in Graphormer：

- Centrality Encoding:
  - develop a Centrality Encoding which assigns each node two real-valued embedding vectors according to its indegree and outdegree.

$$h_i^{(0)} = x_i + z^-_{\deg^-(v_i)} + z^+_{\deg^+(v_i)}$$

- Spatial Encoding:
  - choose ϕ(vi, vj) to be the distance of the shortest path (SPD) between vi and vj.
- Edge Encoding:
  - find the shortest path SP_{ij} = (e1, e2, ..., eN) from vi to vj, and compute an average of the dot-products of the edge feature and a learnable embedding along the path.

$$A_{ij} = \frac{(h_i W_Q)(h_j W_K)^T}{\sqrt{d}} + b_{\phi(v_i,v_j)} + c_{ij}, \text{ where } c_{ij} = \frac{1}{N}\sum_{n=1}^{N} x_{e_n}(w_n^E)^T$$

GRAPH-BERT

Motivation：

- Traditional message passing-based models have limited representation capabilities.
- The inherently interconnected nature precludes large-sized graph parallelization, as memory constraints limit batching across the nodes.
- Existing GNN models have several serious learning performance problem, e.g., suspended animation problem and over-smoothing problem.

Zhang J, Zhang H, Xia C, et al. Graph-bert: Only attention is needed for learning graph representations. arXiv 2020[J]. arXiv preprint arXiv:2001.05140, 2001.

GRAPH-BERT

Part 1: linkless subgraph batching instead of the complete graph

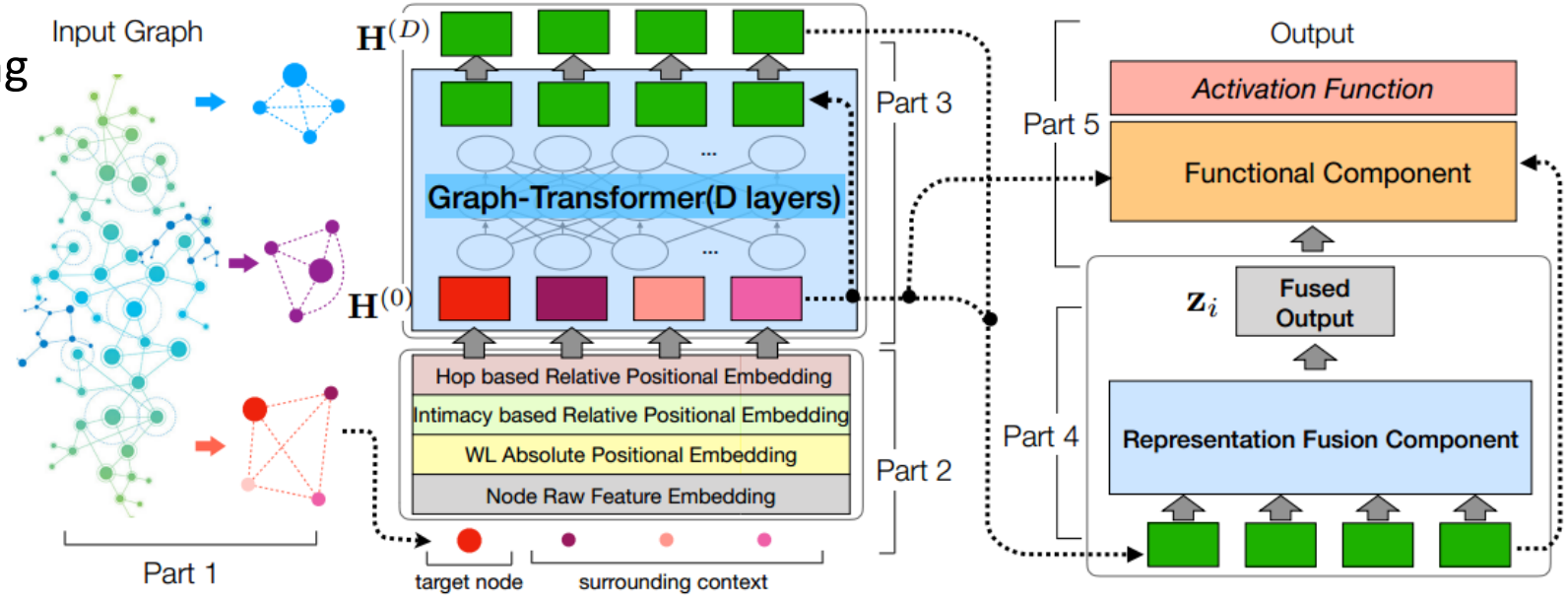
Part 2: Node Input Vector Embeddings

1. raw feature vector embedding
2. Weisfeiler-Lehman absolute role embedding
3. intimacy-based relative positional embedding
4. hop-based relative distance embedding

Part 3: graph transformer based encoder

Part 4: representation fusion

Part 5: functional component



GRAPH-BERT

How to handle large-scale graph input?

- Linkless Subgraph Sampling and Batching
  - Introduce the top-k intimacy sampling approach and trained with linkless subgraph batches sampled from the input graph instead of complete graph

How to deal with insufficient model representation?

- More node-related information as node initial features

1. raw feature vector embedding

$$\mathbf{e}_j^{(x)} = \text{Embed}(\mathbf{x}_j) \in \mathbb{R}^{d_h \times 1}$$

2. Weisfeiler-Lehman absolute role embedding

$$\mathbf{e}_j^{(r)} = \text{Position-Embed}(\text{WL}(v_j))$$

$$= \left[sin\left(\frac{\text{WL}(v_j)}{10000^{\frac{2l}{d_h}}} \right), cos\left(\frac{\text{WL}(v_j)}{10000^{\frac{2l+1}{d_h}}} \right) \right]_{l=0}^{\lfloor \frac{d_h}{2} \rfloor}$$

3. intimacy-based relative positional embedding

$$\mathbf{e}_j^{(p)} = \text{Position-Embed}(\text{P}(v_j)) \in \mathbb{R}^{d_h \times 1}$$

4. hop-based relative distance embedding

$$\mathbf{e}_j^{(d)} = \text{Position-Embed}(\text{H}(v_j; v_i)) \in \mathbb{R}^{d_h \times 1}.$$

$$\mathbf{h}_j^{(0)} = \text{Aggregate}(\mathbf{e}_j^{(x)}, \mathbf{e}_j^{(r)}, \mathbf{e}_j^{(p)}, \mathbf{e}_j^{(d)})$$

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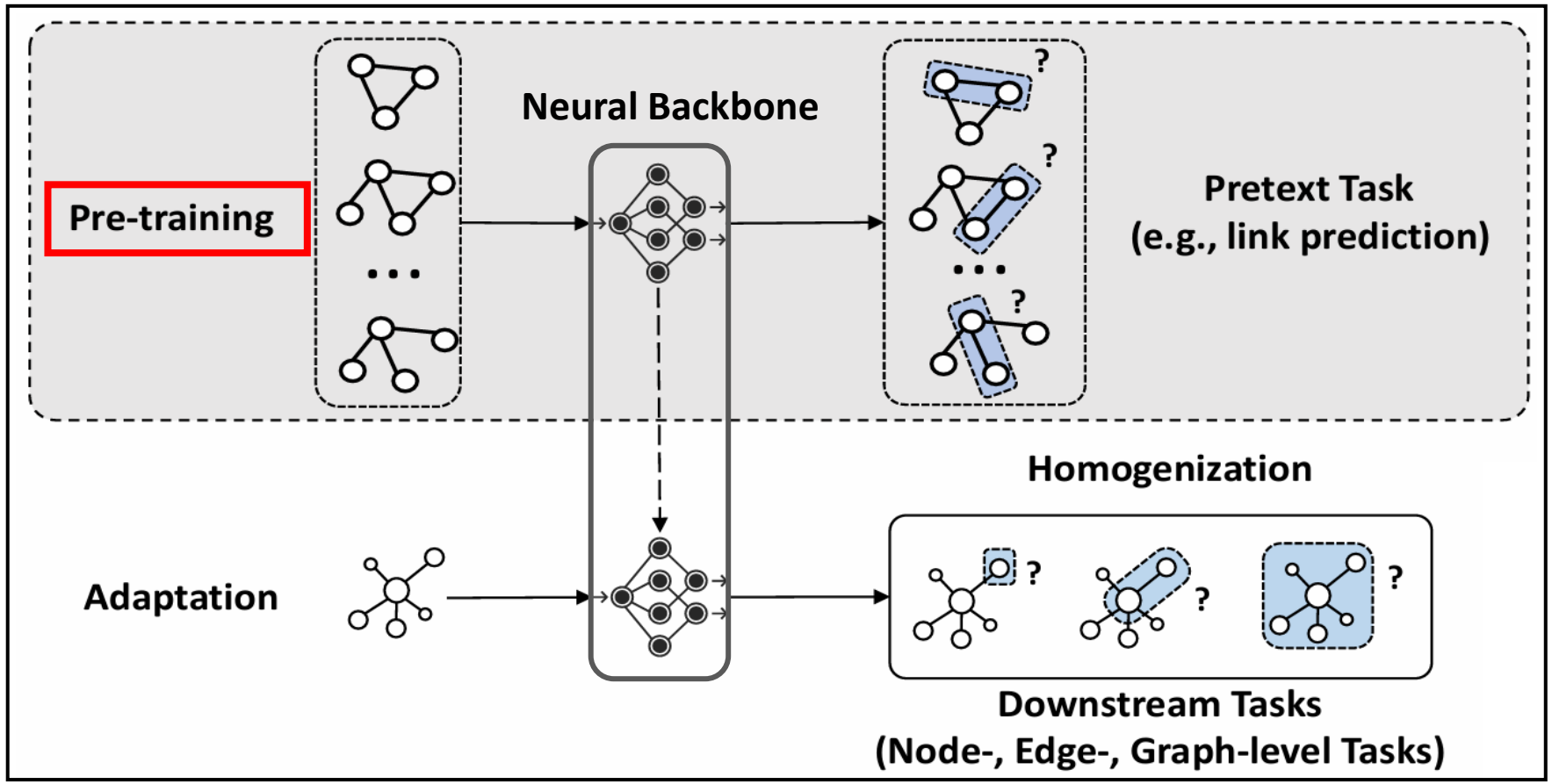

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Pre-training

Pre-training

- Generative methods:
  - graph reconstruction
  - property prediction

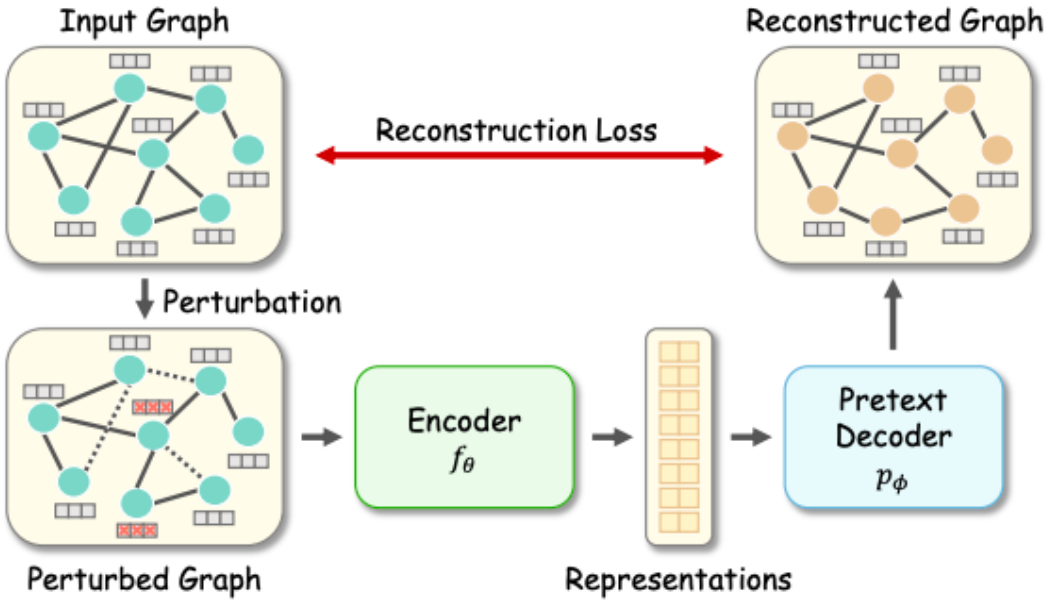
- Contrastive methods:
  - same-scale contrastive learning
  - cross-scale contrastive learning

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.

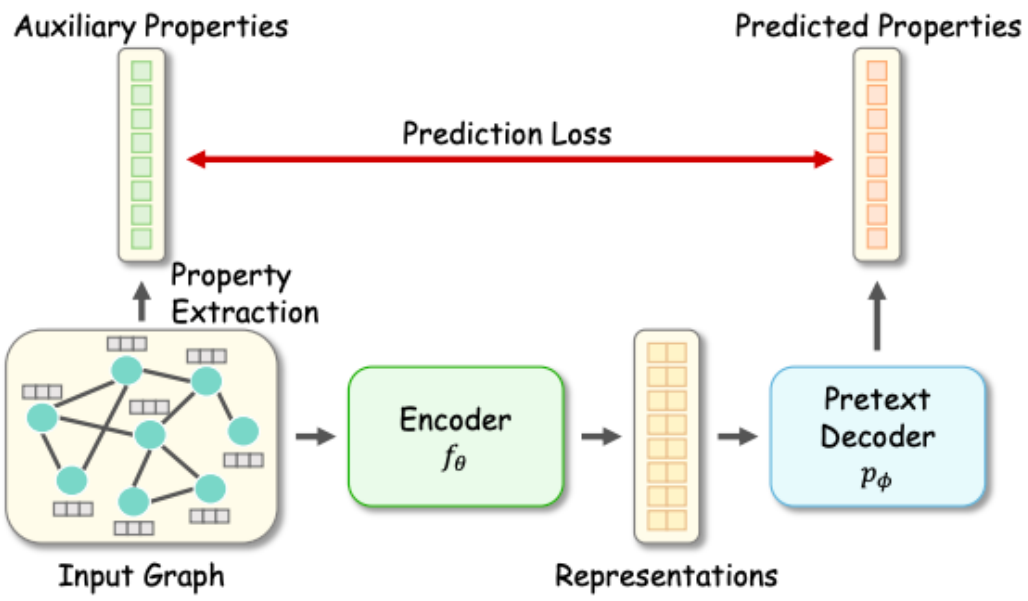
Pre-training

Pre-training

- Generative methods: graph reconstruction, property prediction



graph reconstruction



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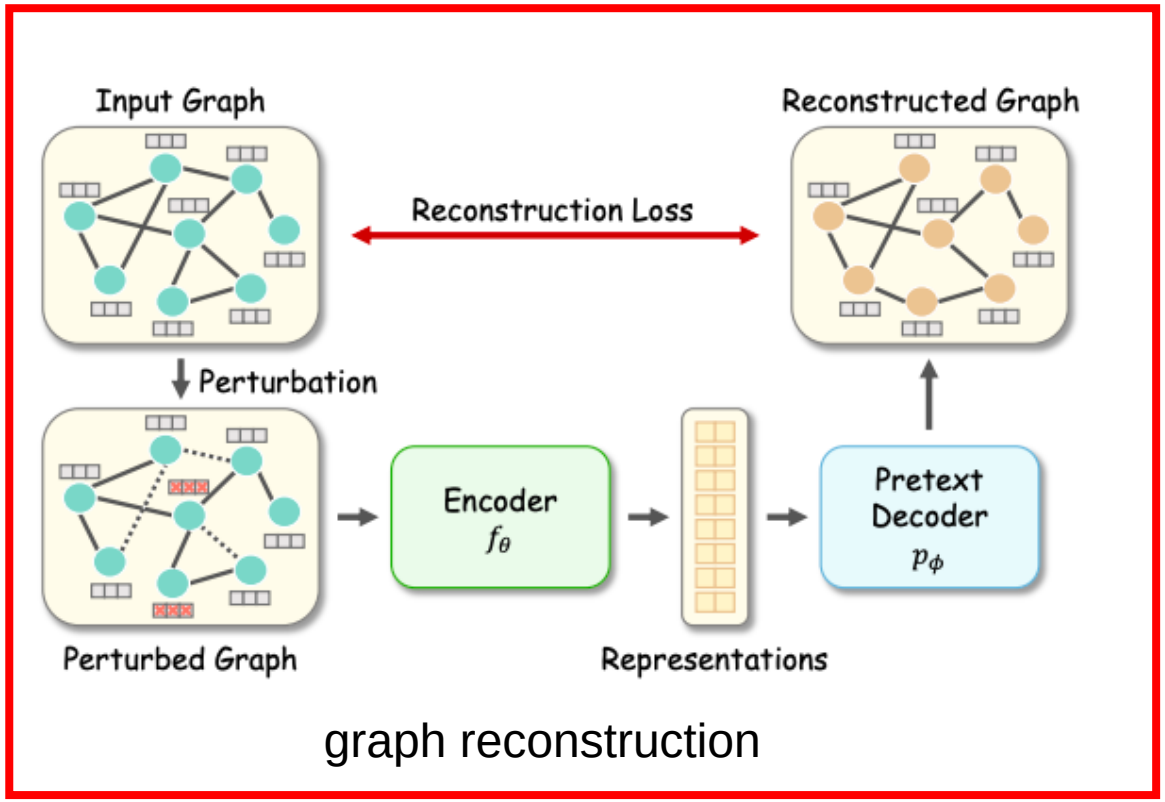

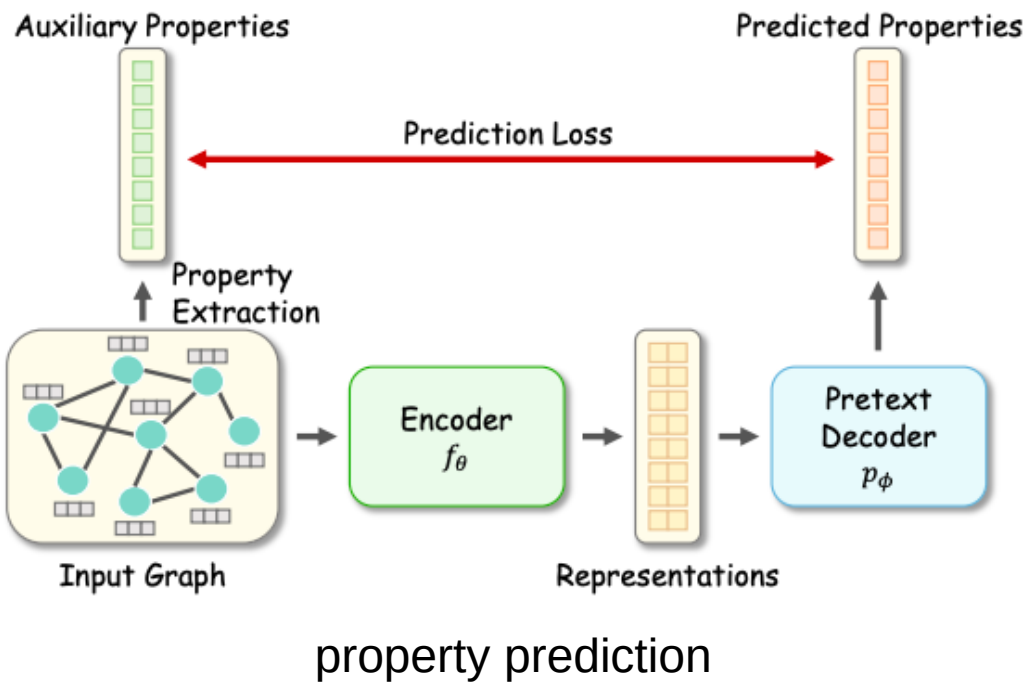

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GPT-GNN

Motivations:

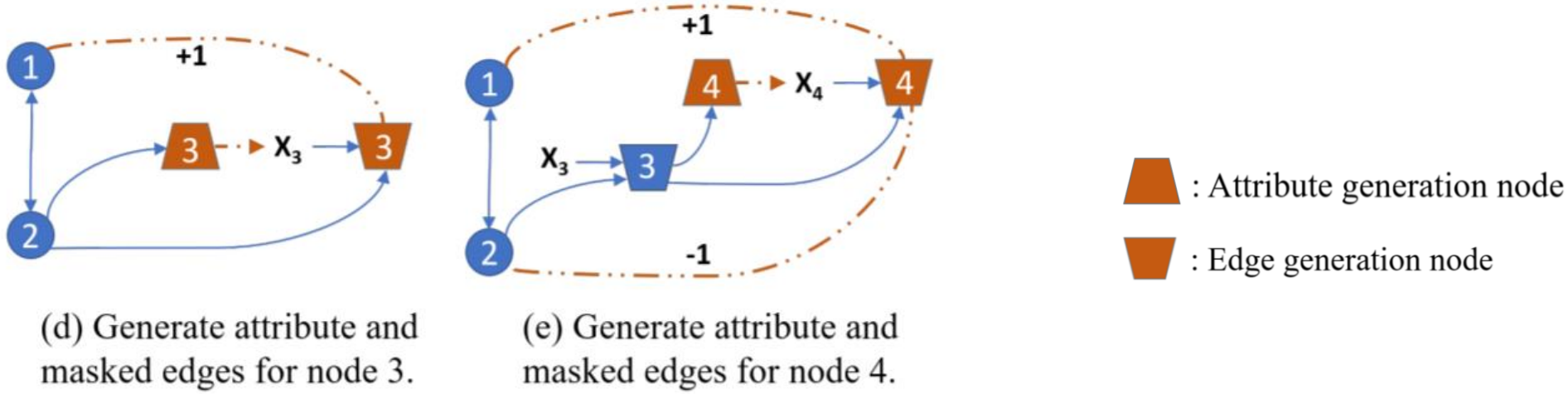
- **Scarcity of Labeled Data**: Adequate labeled data is often unavailable for training GNNs on specific tasks.
- **Proven Success of Pre-training**: Pre-training has significantly enhanced performance in domains like NLP and computer vision.
- **Need for Generalization**: Pre-training GNNs can help them generalize across various tasks with minimal customization.

Hu Z, Dong Y, Wang K, et al. GPT-GNN: Generative pre-training of graph neural networks. KDD2020.

GPT-GNN

Pre-train large-scale graph with **reconstructing** the input graph. Decompose the reconstruction process into two coupled steps:

- Attribute generation: given observed edges, generate **node attributes**
- Edge generation: given observed edges and generated attributes, generate **masked edges**



Hu Z, Dong Y, Wang K, et al. GPT-GNN: Generative pre-training of graph neural networks. KDD2020.

Adaptive Graph Encoder

Motivations:

- Reconstructing the adjacency matrix = contrasting adjacent nodes
- Assumption: A node is similar to its neighbors.

Reasonable?

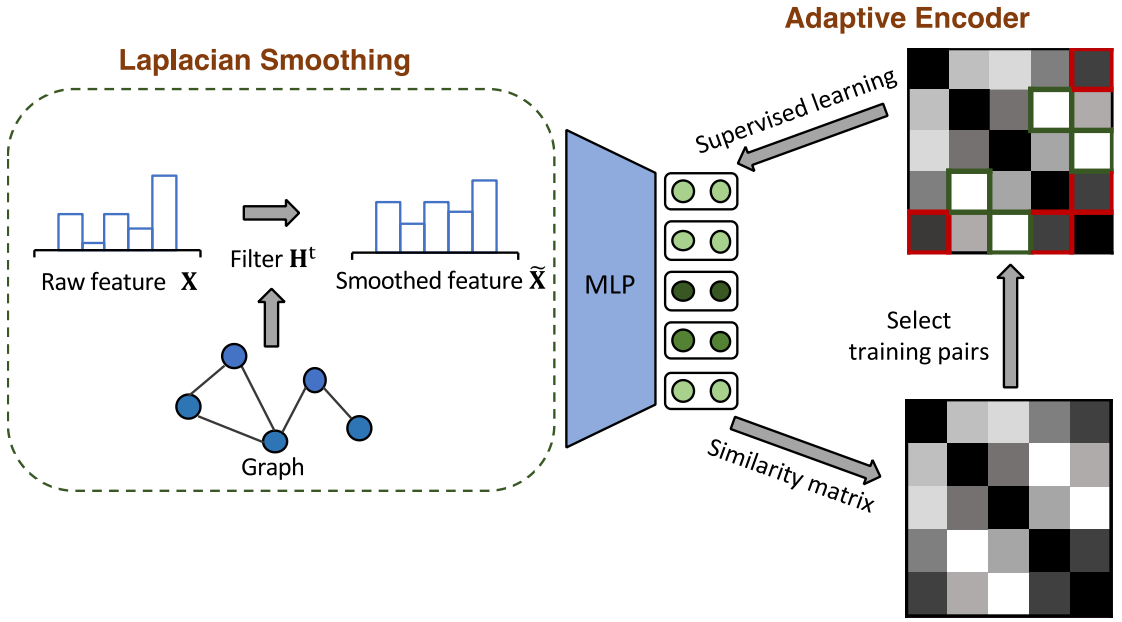
The three main drawbacks of GAE:

- **Entangled Architecture**: Combines multiple layers in a way that complicates training without improving performance.
- **Ineffective Filters**: The graph convolutional filters used are not optimal for filtering out high-frequency noise.
- **Unsuitable Objectives**: The training goals of reconstructing adjacency and feature matrices are not practical, as they can either overlook key data or retain unwanted noise.

Cui G, Zhou J, Yang C, et al. Adaptive graph encoder for attributed graph embedding. KDD 2020

Adaptive Graph Encoder

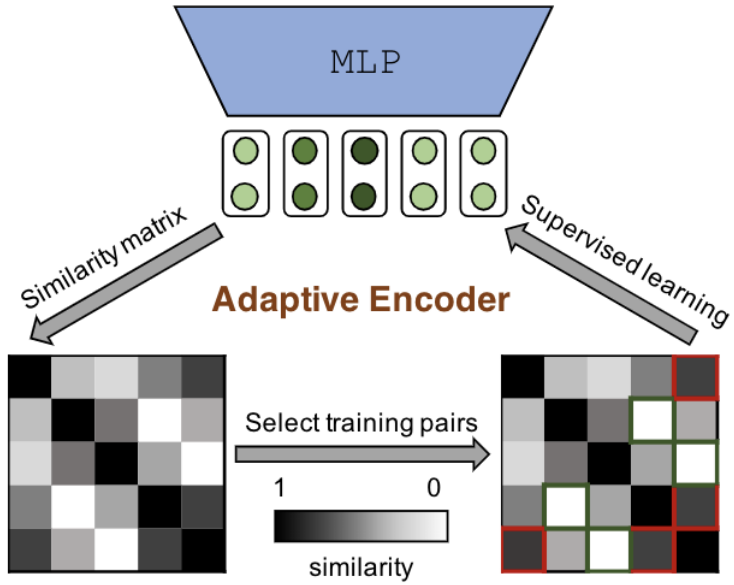
- **Laplacian Smoothing**: Design appropriate Laplacian smoothing filters to filter out high-frequency noise.
- **Adaptive Encoder**: Adaptively select training node pairs from the node similarity and adjust graph representations accordingly.



Adaptive Graph Encoder

- How to set training objectives to learn graph representations?
  - The adjacency matrix records only one-hop structural information.
  - Smoothed features or trained representations integrate both structural and feature information.
- Adaptively select training node pairs:
  - High similarity pairs as positive examples.
  - Low similarity pairs as negative examples.

- Select Strategy
  - Calculate the cosine similarity matrix S.
  - Sort all node pairs and select those whose similarity is above/below a certain threshold.
  - Dynamically update the threshold.



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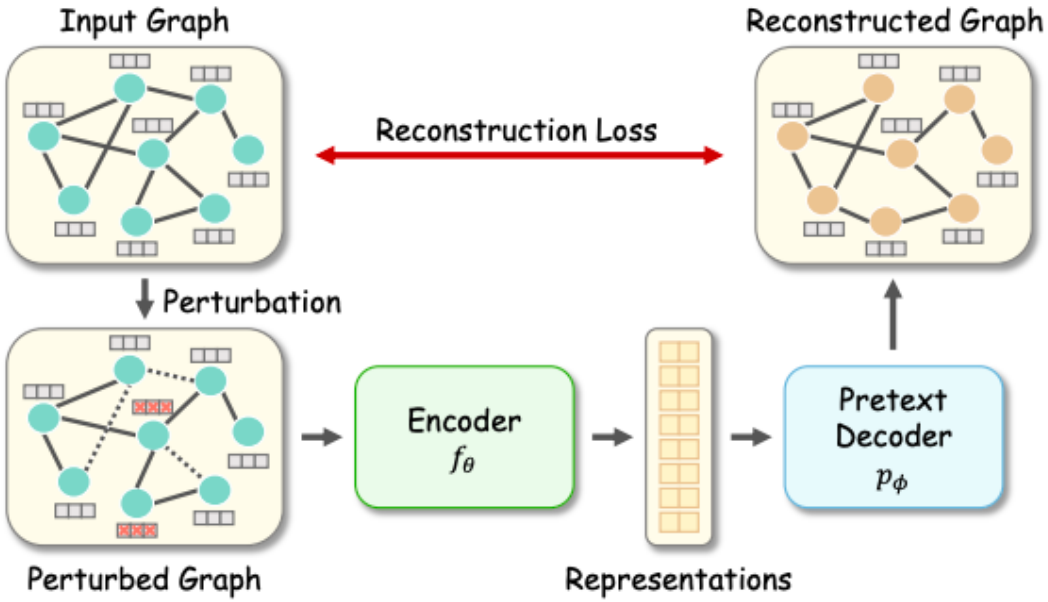
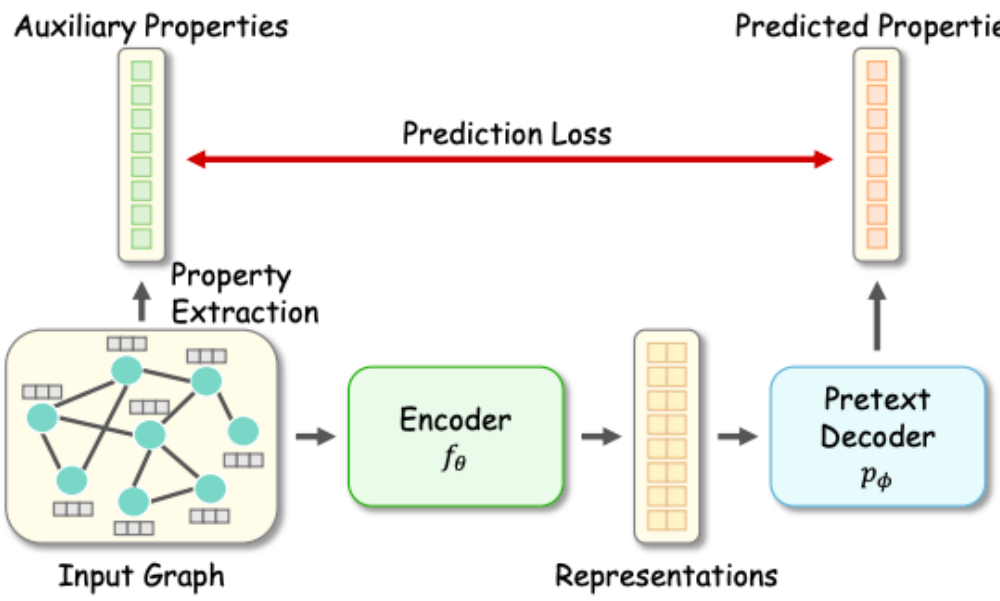


graph reconstruction



property prediction

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GraphMAE

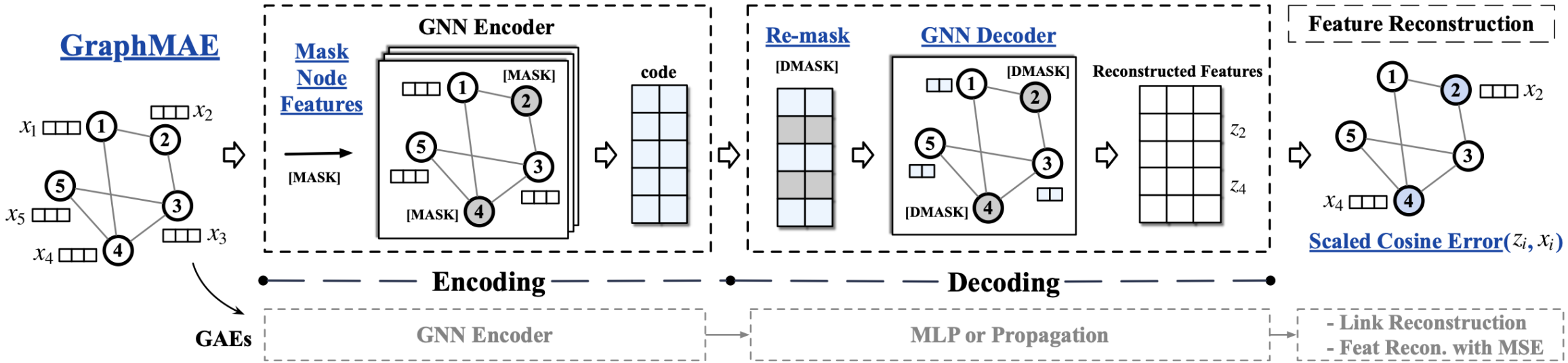
Motivations:

- **Lagging Development of GAEs**: GAEs lag behind contrastive methods in critical tasks like node and graph classifications, highlighting a need for enhanced models.
- **Challenges in Current GAE Approaches**: Existing GAEs struggle with issues like non-robust feature reconstruction and sensitivity to MSE, prompting the need for methodological improvements.
- **Decoder Limitations**: The simple MLP decoders commonly used in GAEs are inadequate for complex graph data, suggesting a need for more expressive architectures.

Hou Z, Liu X, Cen Y, et al. Graphmae: Self-supervised masked graph autoencoders[C]//Proceedings of the 28th ACM SIGKDD Conference on Knowledge Discovery and Data Mining.

GraphMAE

Masked Feature Reconstruction: Focuses on node feature reconstruction with masking, proven effective in enhancing performance.
Scaled Cosine Error: Uses a scaled cosine error for better handling of feature magnitude variations and sample difficulty imbalances.
Re-mask Decoding: Employs re-masking of encoded node embeddings to improve decoding accuracy.
Advanced Decoder Architecture: Incorporates complex GNNs in the decoder for improved expressiveness.



GROVER

Motivations:

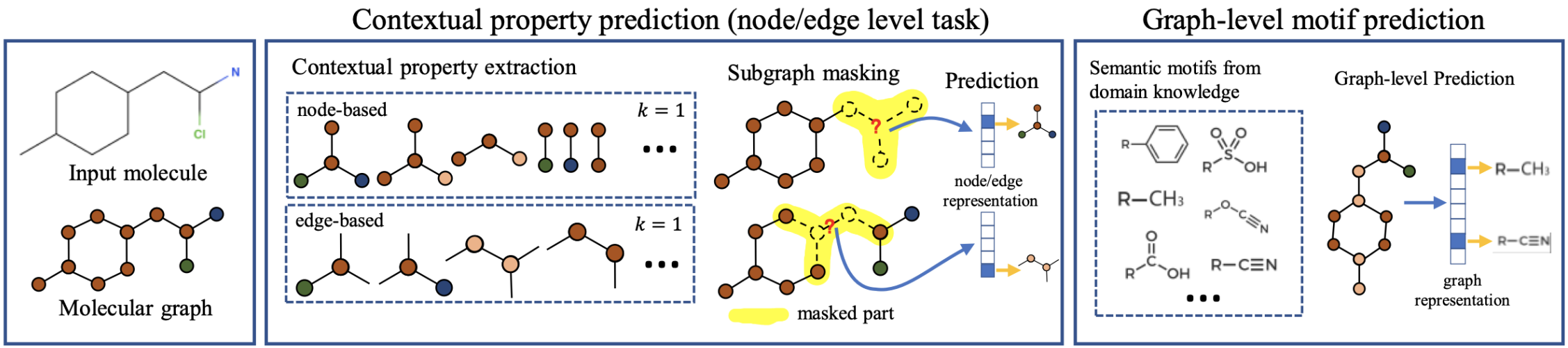
- **Scarcity of Labeled Data**: There is a significant lack of labeled molecular data, making it challenging to apply traditional supervised learning effectively in drug discovery.
- **Limitations of Current Methods**: Existing molecular representation methods, like SMILES, fail to adequately capture the complex topological information of molecules.
- **Need for Novel Strategies**: There is a pressing need for novel computational strategies that can efficiently exploit vast amounts of unlabeled molecular data to improve prediction accuracy and model generalization.

Yu Rong, Yatao Bian, et al. Self-Supervised Graph Transformer on Large-Scale Molecular Data. NIPS2020.

GROVER

Designed self-supervised tasks in node-, edge- and graph-level, learn rich **structural** and **semantic** information of molecules

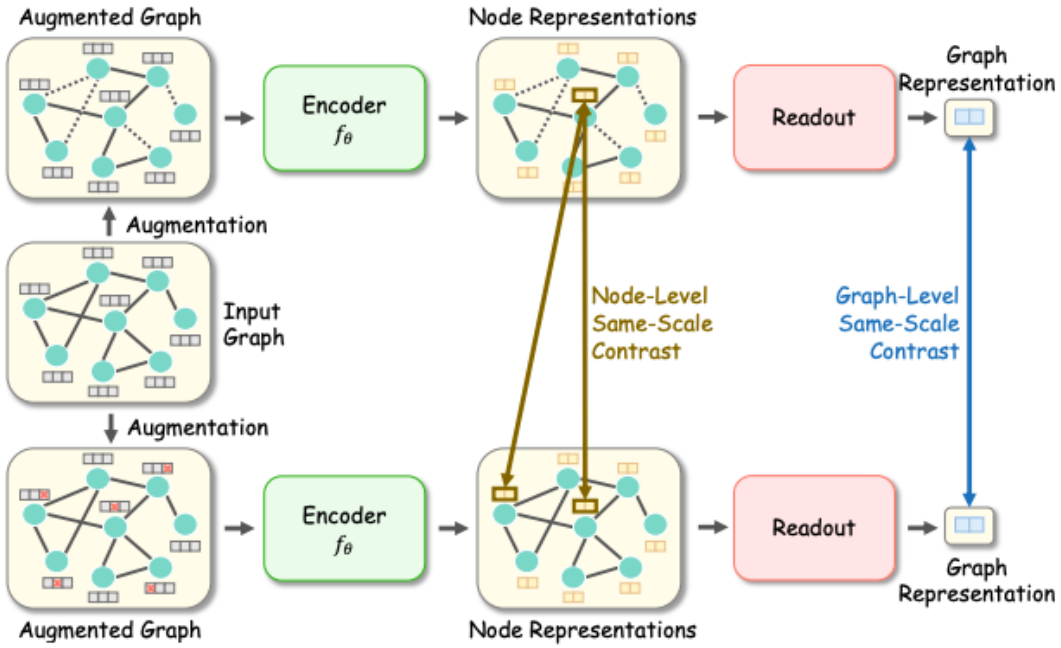
- Contextual property prediction: predict **masked node/edge** attributes set
- Motif prediction : predict the classes of **the motif** that occur in a given molecule



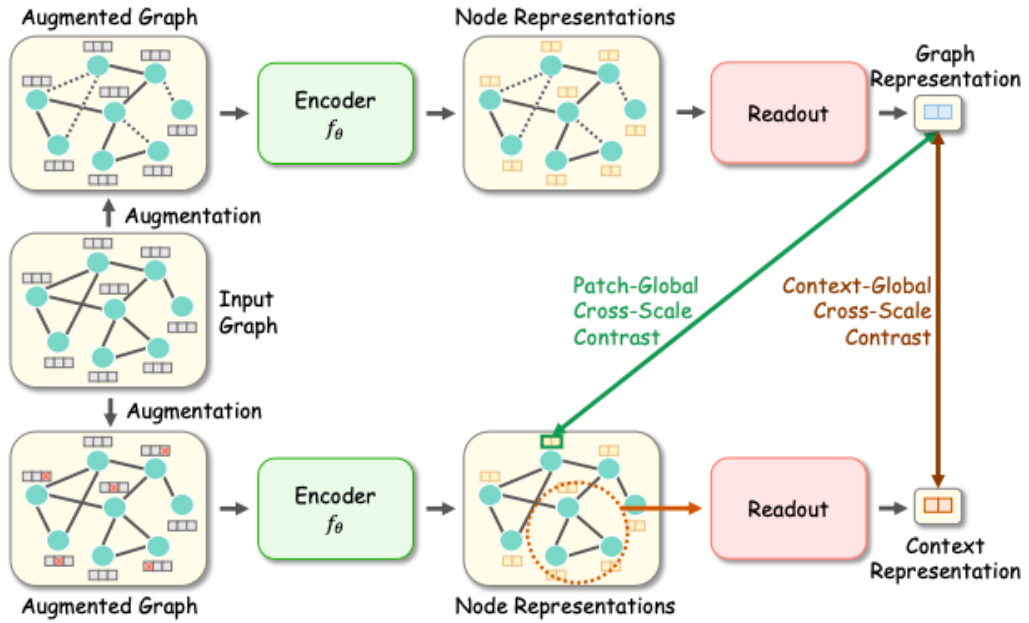
GNN-based Models

Pre-training

- Contrastive methods: same-scale contrastive learning, cross-scale contrastive learning



same-scale contrastive learning



cross-scale contrastive learning

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GNN-based Models

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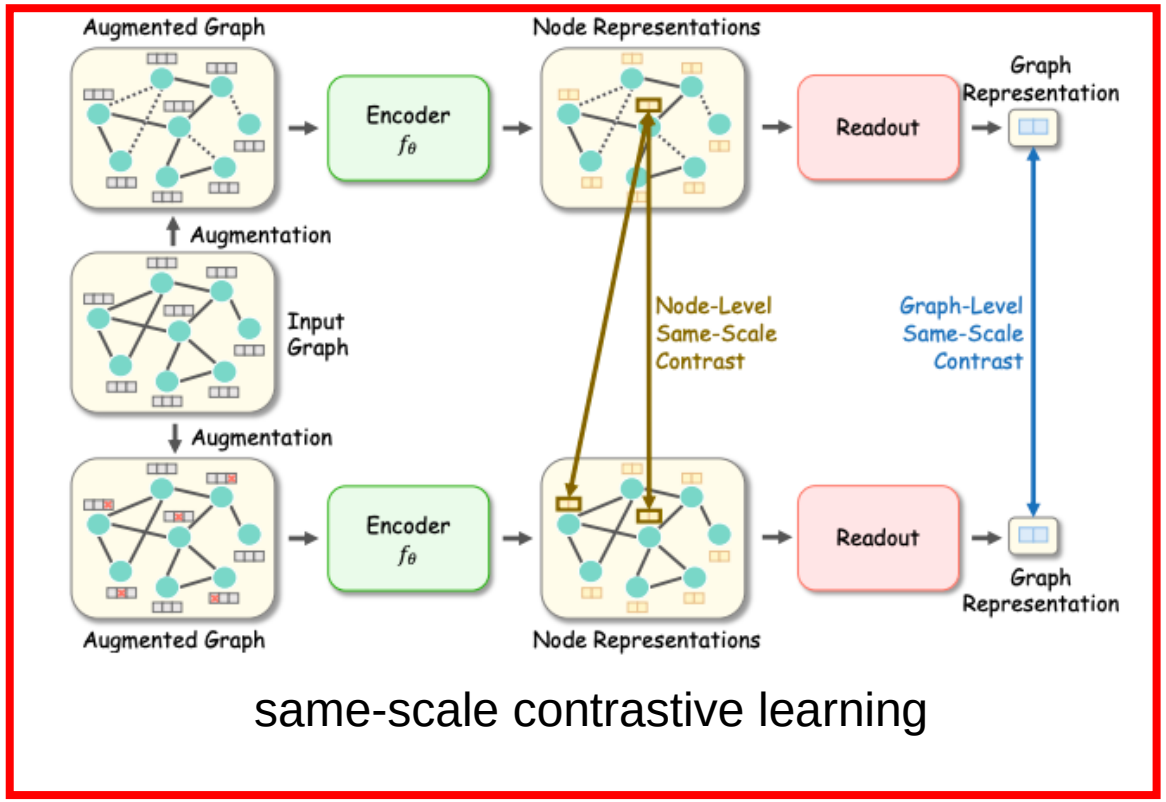
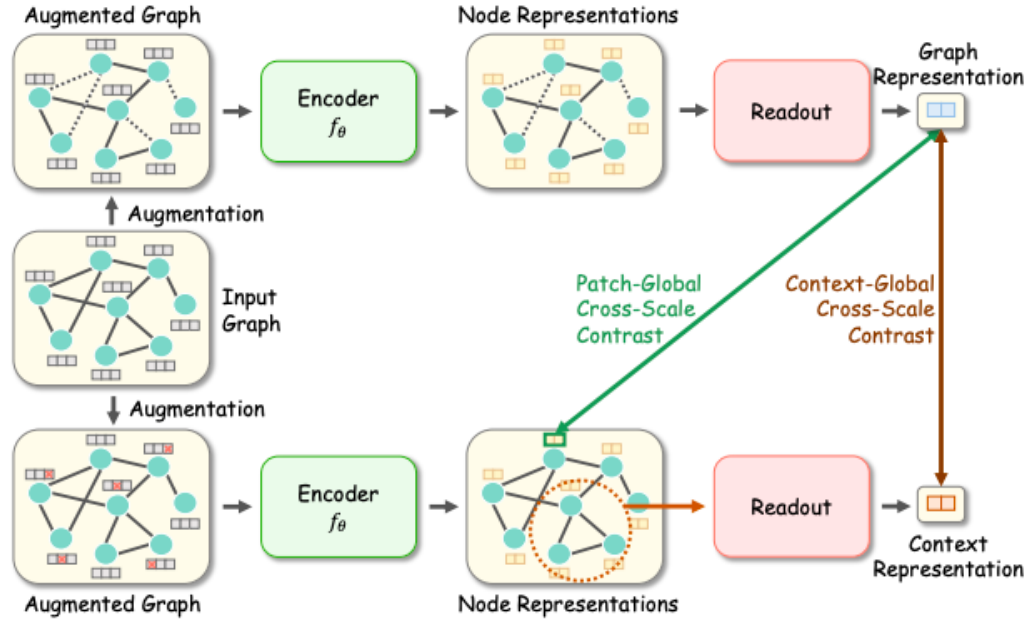


same-scale contrastive learning



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.

GraphCL

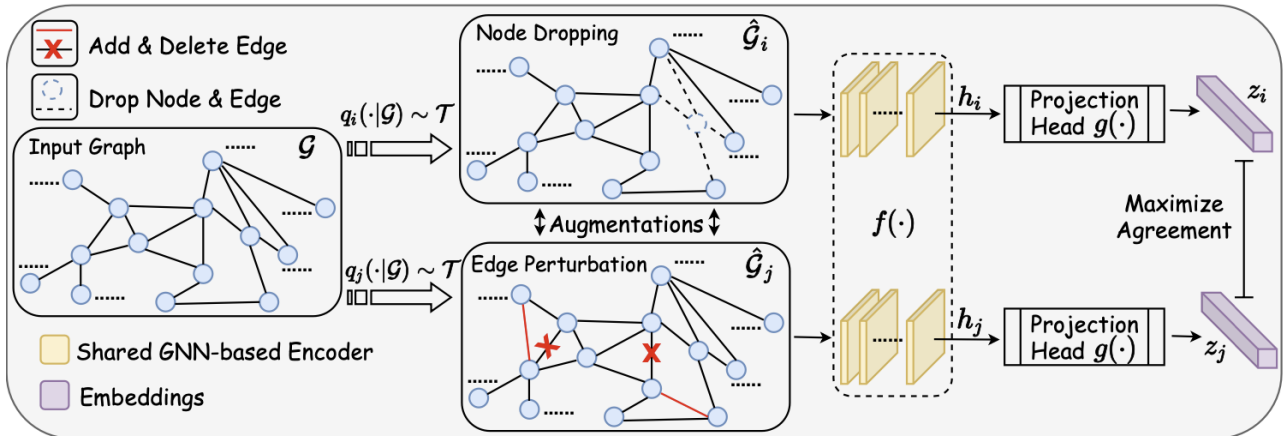
Motivations

- **Label Scarcity:** In fields like biology and chemistry, acquiring labels is costly and slow, making pre-training a valuable strategy to enhance GNNs, akin to its use in CNNs.
- **Complex Graph Data:** The diverse and complex nature of graph data makes designing effective pre-training schemes challenging, as simple methods like adjacency reconstruction may fall short.
- **Contrastive Learning Potential:** Contrastive learning could potentially overcome the limitations of proximity-focused pre-training by promoting feature consistency across different views.

Yuning You, Tianlong Chen, Yongduo Sui, et al. Graph Contrastive Learning with Augmentations. NeurIPS2020

GraphCL

Design four types of **graph augmentations** to incorporate various impacts in four different settings: semi-supervised, unsupervised, transfer learning and adversarial attacks.



$$\ell_n = -\log \frac{\exp(\text{sim}(\boldsymbol{z}_{n,i}, \boldsymbol{z}_{n,j})/\tau)}{\sum_{n'=1,n' \neq n}^{N} \exp(\text{sim}(\boldsymbol{z}_{n,i}, \boldsymbol{z}_{n',j})/\tau)}$$

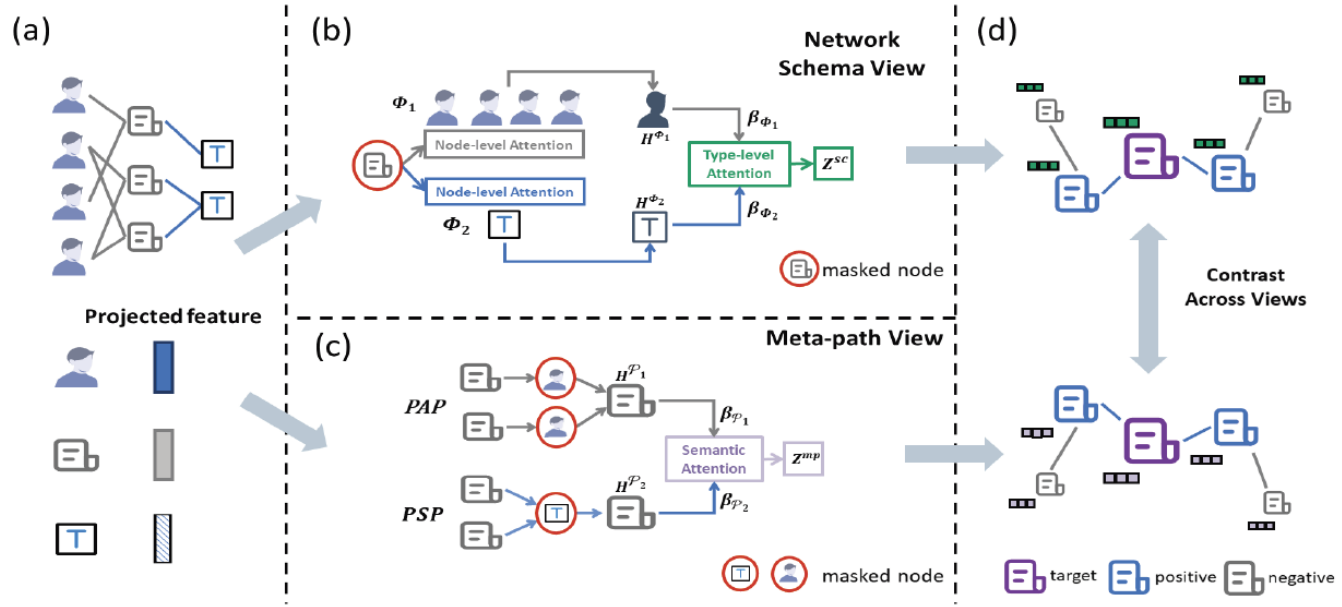
Contrast augmentation of same&diffferent graphs

Data augmentation	Type	Underlying Prior
Node dropping	Nodes, edges	Vertex missing does not alter semantics.
Edge perturbation	Edges	Semantic robustness against connectivity variations.
Attribute masking	Nodes	Semantic robustness against losing partial attributes.
Subgraph	Nodes, edges	Local structure can hint the full semantics.

HeCo

Core idea:

- Two views of a HIN (network schema and meta-path views) are proposed to capture both of local and high-order structures simultaneously.
- The cross-view contrastive learning is proposed to extract the positive and negative embeddings from two views.
- The two views to collaboratively supervise each other and finally learn high-level node embeddings.



Wang X, Liu N, Han H, et al. Self-supervised heterogeneous graph neural network with co-contrastive learning. KDD 2021

HeCo

Network Schema View Guided Encoder

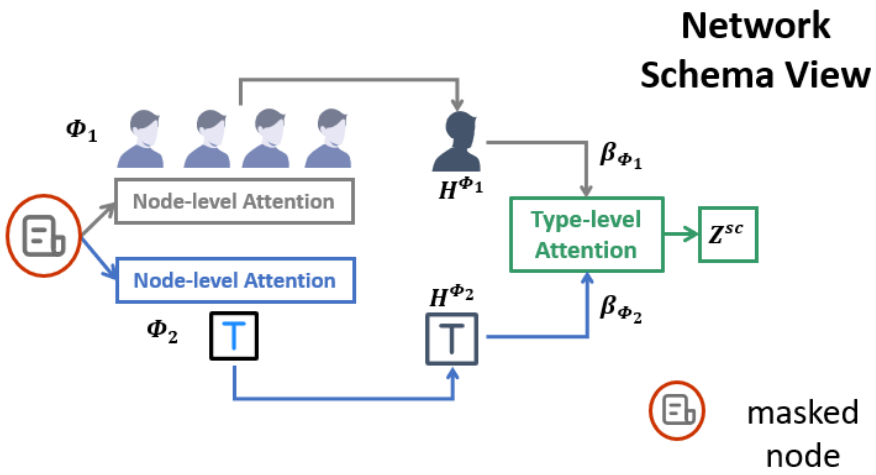
Node-level attention

For target paper

1. randomly sample Φ_m-type neighbors with threshold T_{Φ_m}
2. aggregate them with attention to get embedding of type Φ_m

Type-level aggregation

Aggregate different type of nodes with attention mechanism



Meta-path View Guided Encoder

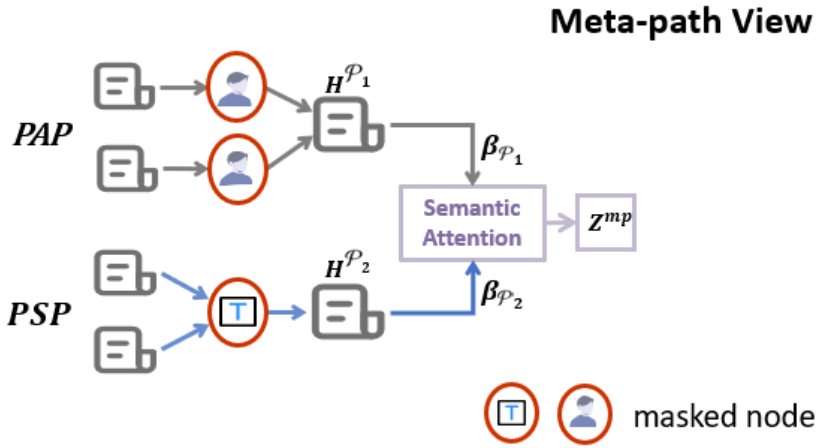
Meta-path specific GCN

For target paper

1. find its neighbors based on different meta-paths
2. aggregate them with meta-path based vanilla GCN

Semantic-level aggregation

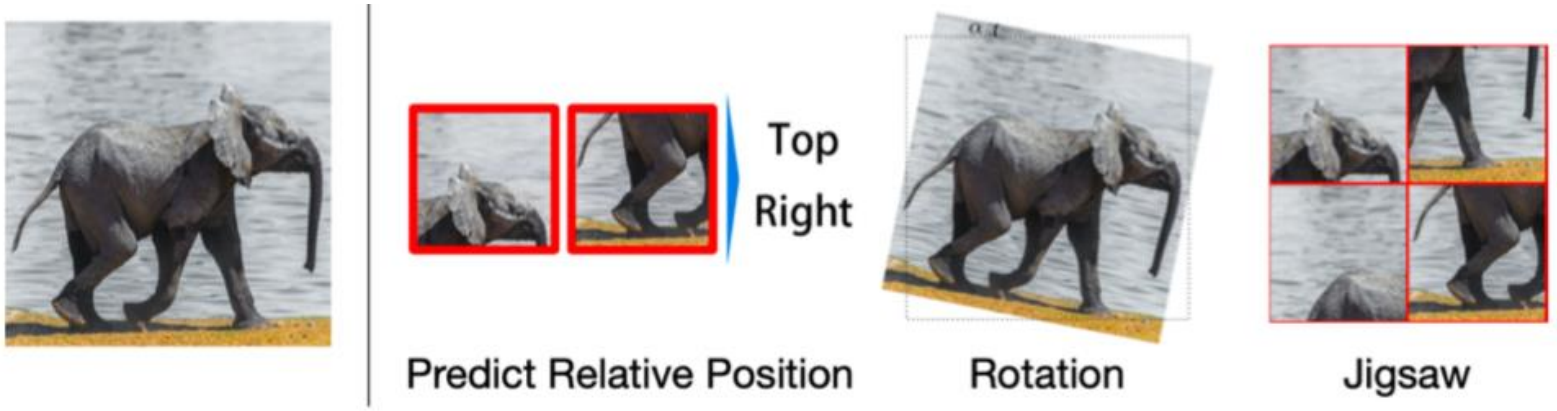
Aggregate embedding under different meta-path with attention mechanism



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?

MA-GCL

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.

MA-GCL

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

MA-GCL

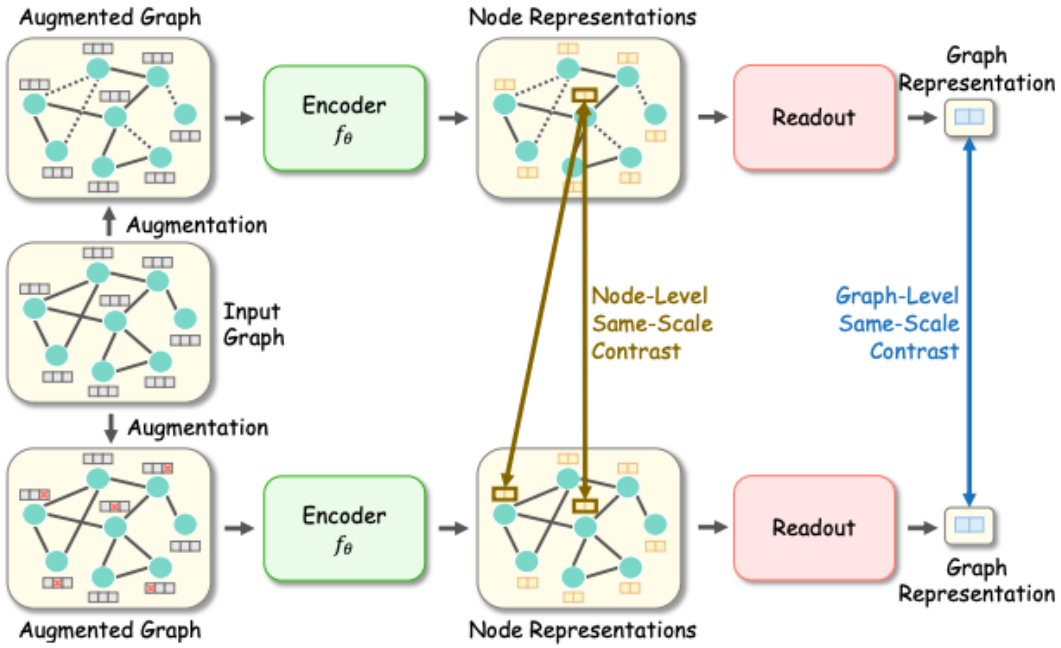
We conducted extensive experiments on node/graph classification/clustering.

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**

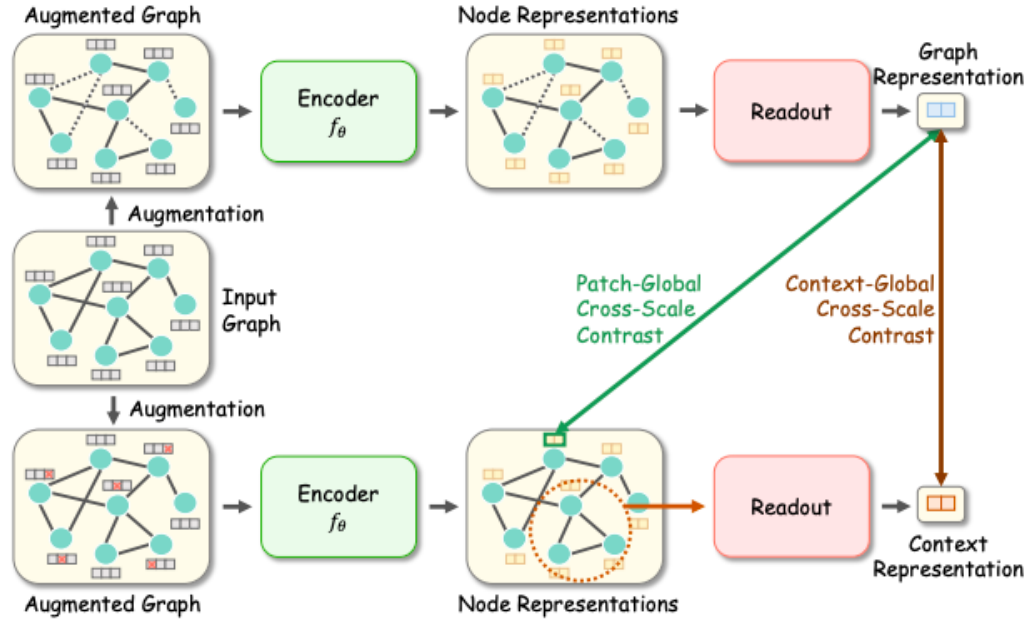
GNN-based Models

Pre-training

- 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.

Deep Graph Infomax

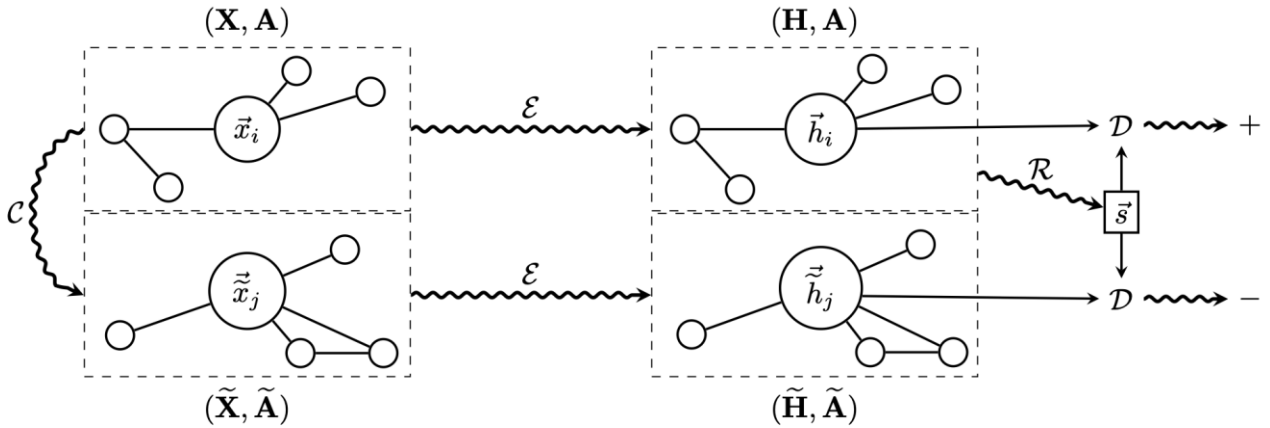
Motivations:

- **Label Scarcity**: Most real-world graph data lacks labels, restricting the use of supervised methods.
- **Structure Discovery**: Unsupervised learning is vital for uncovering new structures in large-scale graphs.
- **Current Method Limitations**: Existing methods like random walks over-emphasize proximity and may neglect broader structural details.

Veličković P, Fedus W, Hamilton W L, et al. Deep Graph Infomax[C]//ICLR. 2018.

Deep Graph Infomax

- **Node Representation**: GCN generates a representation for each node in the graph.
- **Graph Representation**: The global representation of the graph is produced by aggregating all node representations, typically through summation or averaging.
- **Negative Sampling**: Perturbed versions of the graph are generated, for example, by shuffling node features or edges to create negative samples.
- **Maximization of Mutual Information**: The network is trained by maximizing the mutual information between node representations and the global representation in the positive samples (original graph) and minimizing it in the negative samples (perturbed graph).

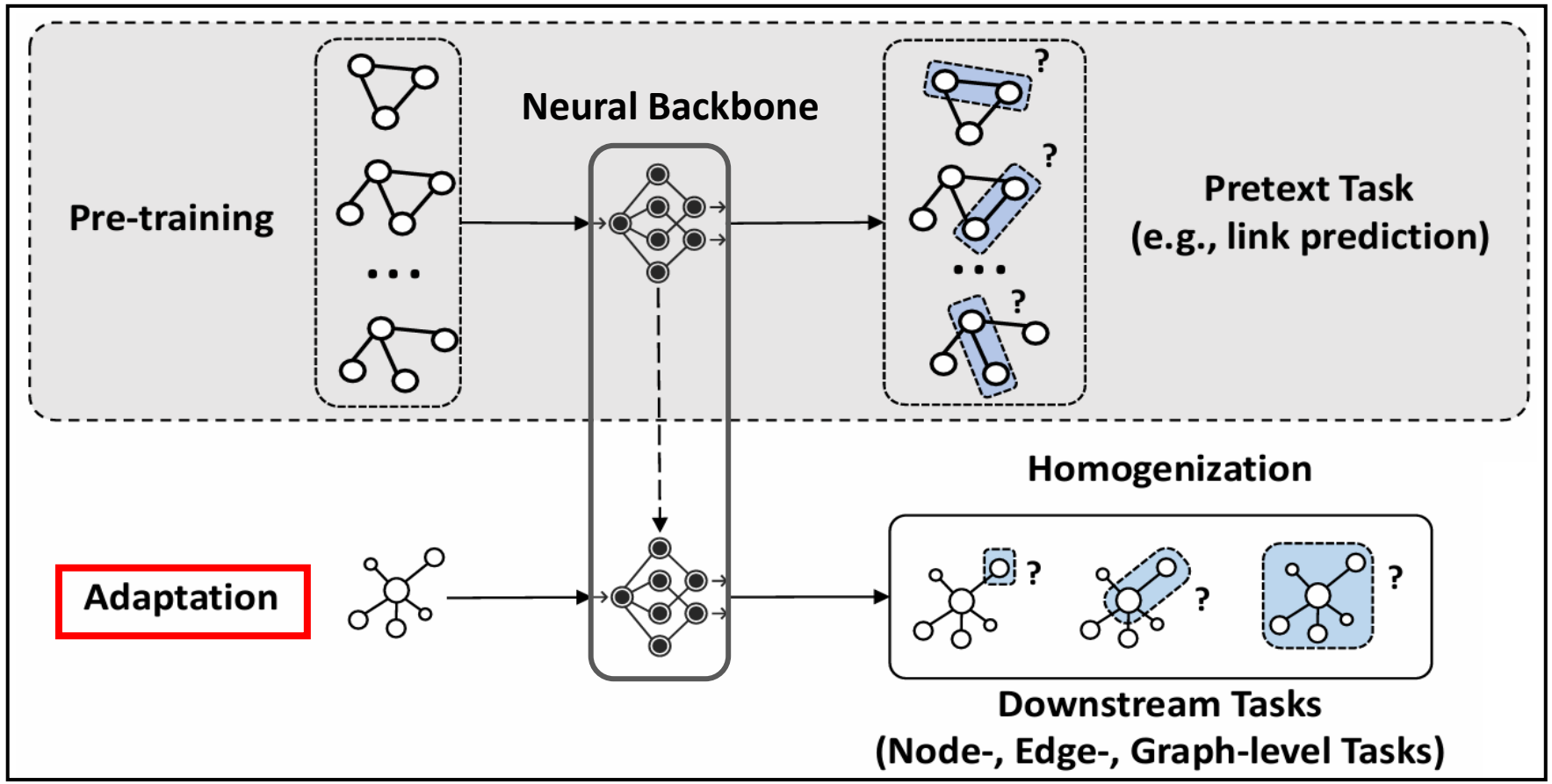


GNN-based Methods

Backbone： No unified architecture

（Message Passing/Graph Transformer）

Paradigm： Pre-training + Adaptation

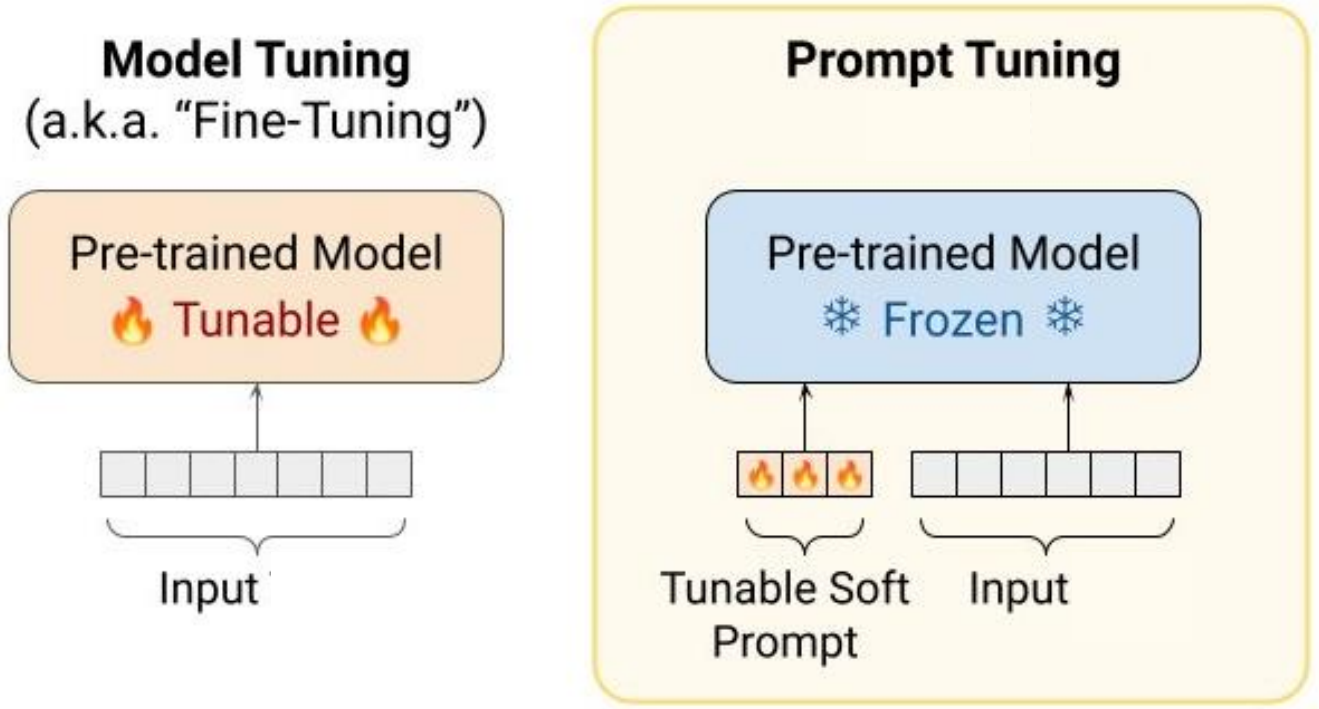


Jiawei Liu, Cheng Yang, Zhiyuan Lu, Junze Chen, Yibo Li, Mengmei Zhang, Ting Bai, Yuan Fang, Lichao Sun, Philip S. Yu, Chuan Shi. Towards Graph Foundation Models: A Survey and Beyond. arXiv 2023

Adaptation

Downstream Adaptation

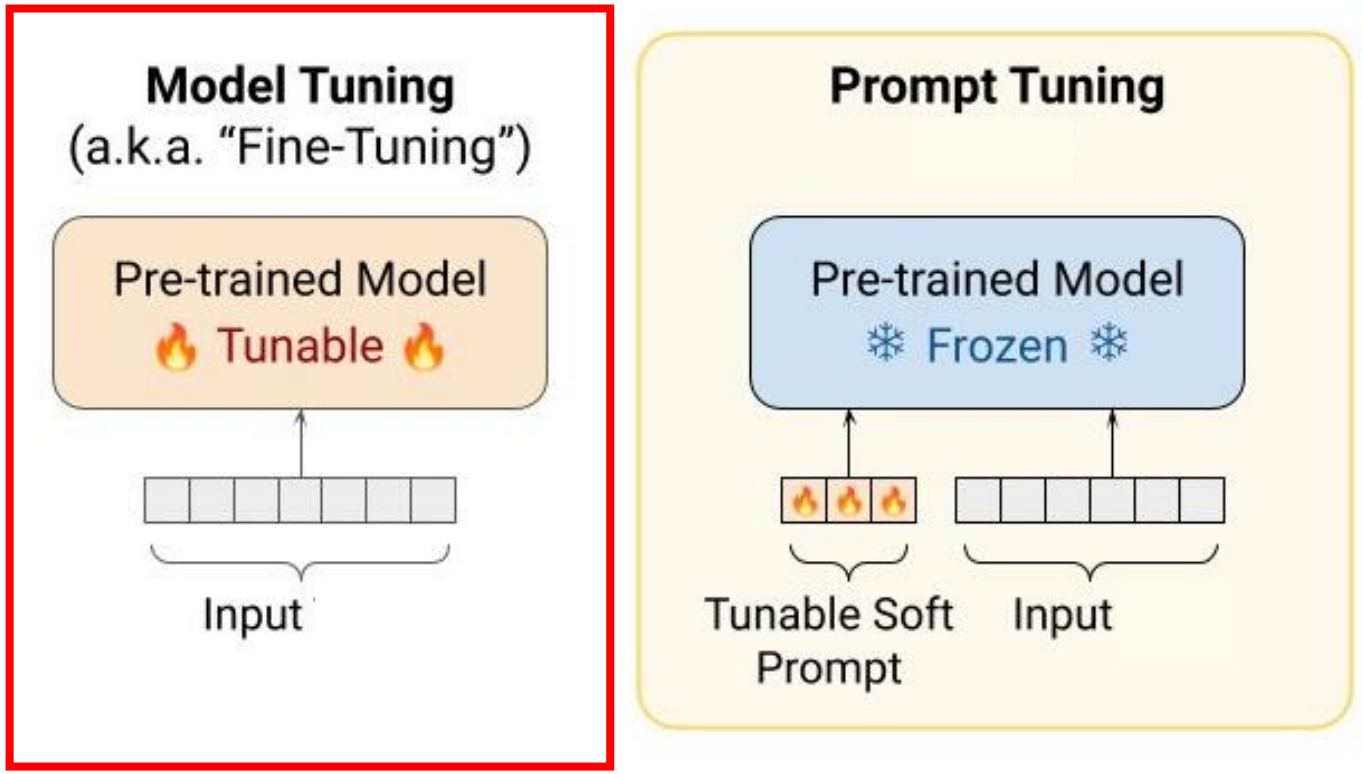
- Fine-tuning: keep input graph intact, modify model parameters accordingly
- Prompt-tuning: keep pre-trained model intact, modify input graph or output embedding



Adaptation

Downstream Adaptation

- Fine-tuning: keep input graph intact, modify model parameters accordingly
  - Parameter-efficient Fine-tuning (PEFT): only tune a small portion of parameters

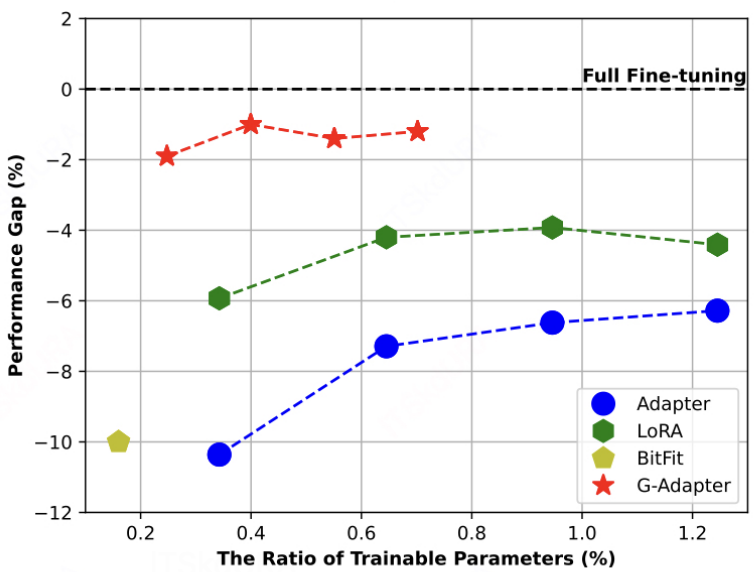


G-Adapter

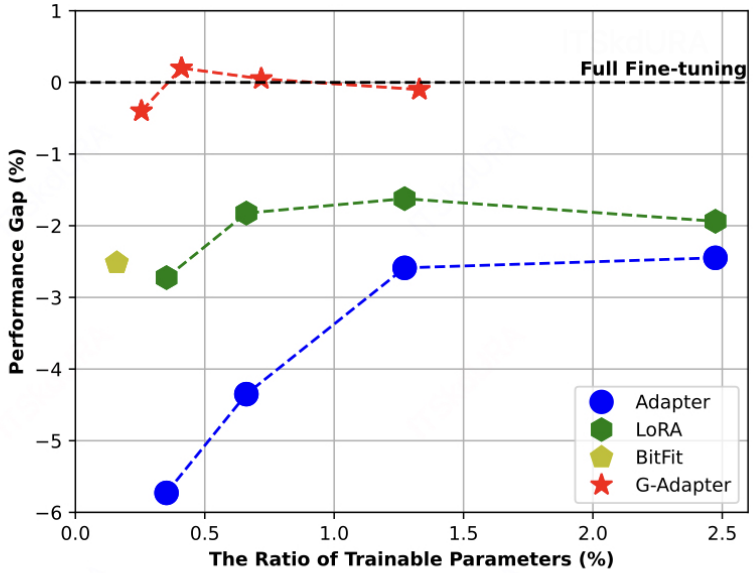
Can PEFTs from the language domain be transferred directly to graph-based tasks?

- There is a significant gap between traditional PEFTs and full fine-tuning, especially on large-scale datasets.

How to design a graph-specific PEFT method?



(a) On large-scale datasets.



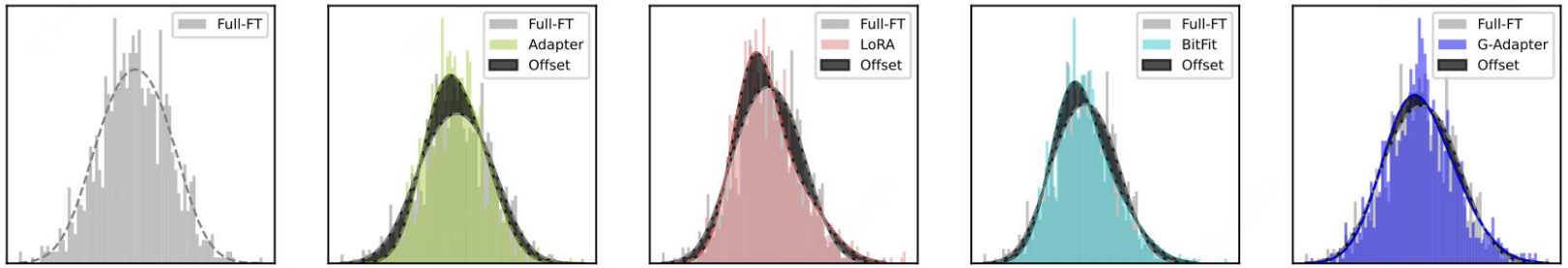
(b) On small-scale datasets.

Gui, A., Ye, J., & Xiao, H. G-adapter: Towards structure-aware parameter-efficient transfer learning for graph transformer networks. AAAI2024

G-Adapter

Method

- Exploration in this paper reveals the feature distribution shift issue due to the absence of graph structure in the fine-tuning process.
- To alleviate these concerns, a novel structure-aware PEFT method, G-Adapter, is proposed, which leverages graph convolution operation to introduce graph structure as the inductive bias to guide the updating process.
- They apply the low-rank decomposition to the learnable weights, which makes G-Adapter highly lightweight.



AdapterGNN

Motivation

- Delta tuning improves the traditional fine-tuning in the catastrophic forgetting of pre-trained knowledge problem and overfitting problem.

How to effectively utilize the advantages of delta tuning while preserving the expressivity of GNNs?

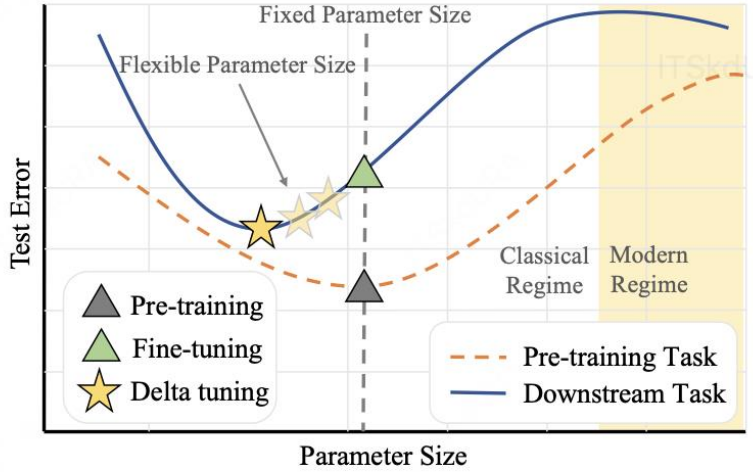
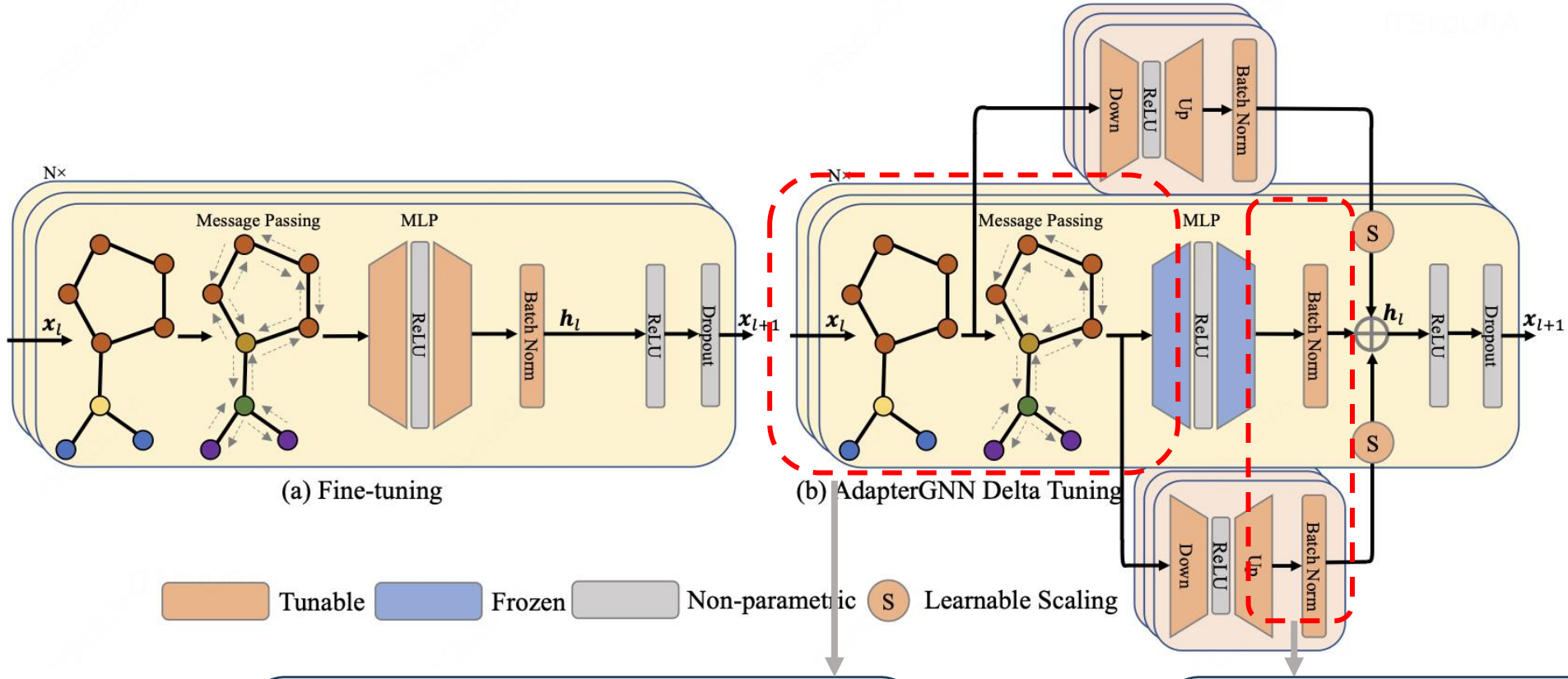


Figure 1: A large model is often employed for pre-training ▲ when sufficient data is available. However, for downstream tasks with limited data, a smaller model is optimal in the classical regime. Compared with fine-tuning ▲, delta tuning ★ preserves expressivity while reducing the size of parameter space, leading to lower test error.

Li, S., Han, X., & Bai, J. AdapterGNN: Parameter-Efficient Fine-Tuning Improves Generalization in GNNs. AAAI2024

AdapterGNN



These adapters utilize bottleneck architecture to significantly reduce the number of tunable parameters by reducing intermediate dimensions.

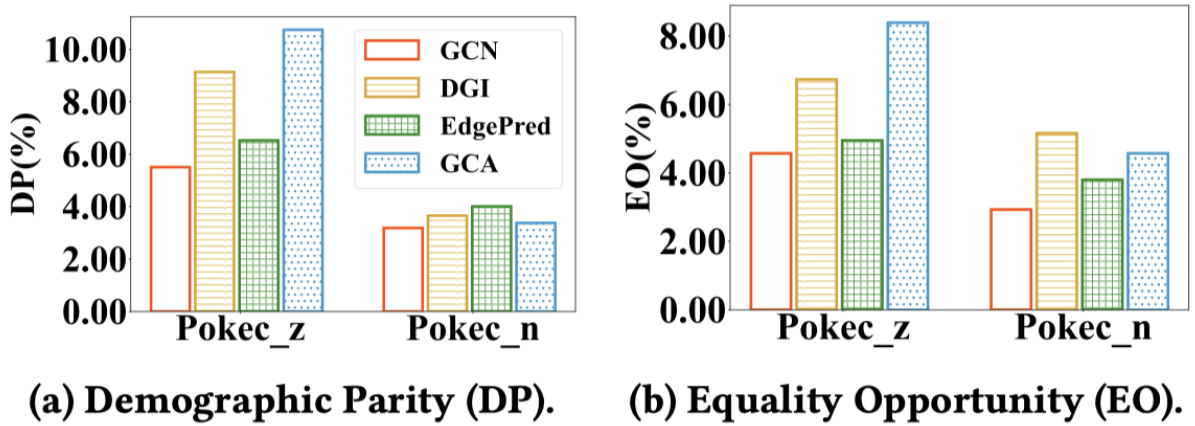
AdapterGNN introduces trainable BN layers in each adapter to maintain consistency with the output of the backbone network.

GraphPAR

Background

- Recent works have demonstrated that pre-trained language models tend to inherit bias from pre-training corpora.
- Pre-trained Graph Models(PGMs) can well capture semantic information on graphs during the pre-training phase, which inevitably contains sensitive attribute semantics.

How to improve the fairness of PGMs?



(a) Demographic Parity (DP). **(b) Equality Opportunity (EO).**

Zhang, Z., Zhang, M., Yu, Y., Yang, C., Liu, J., & Shi, C. Endowing Pre-trained Graph Models with Provable Fairness. WWW2024

GraphPAR

Existing fair methods is inflexible and inefficient.

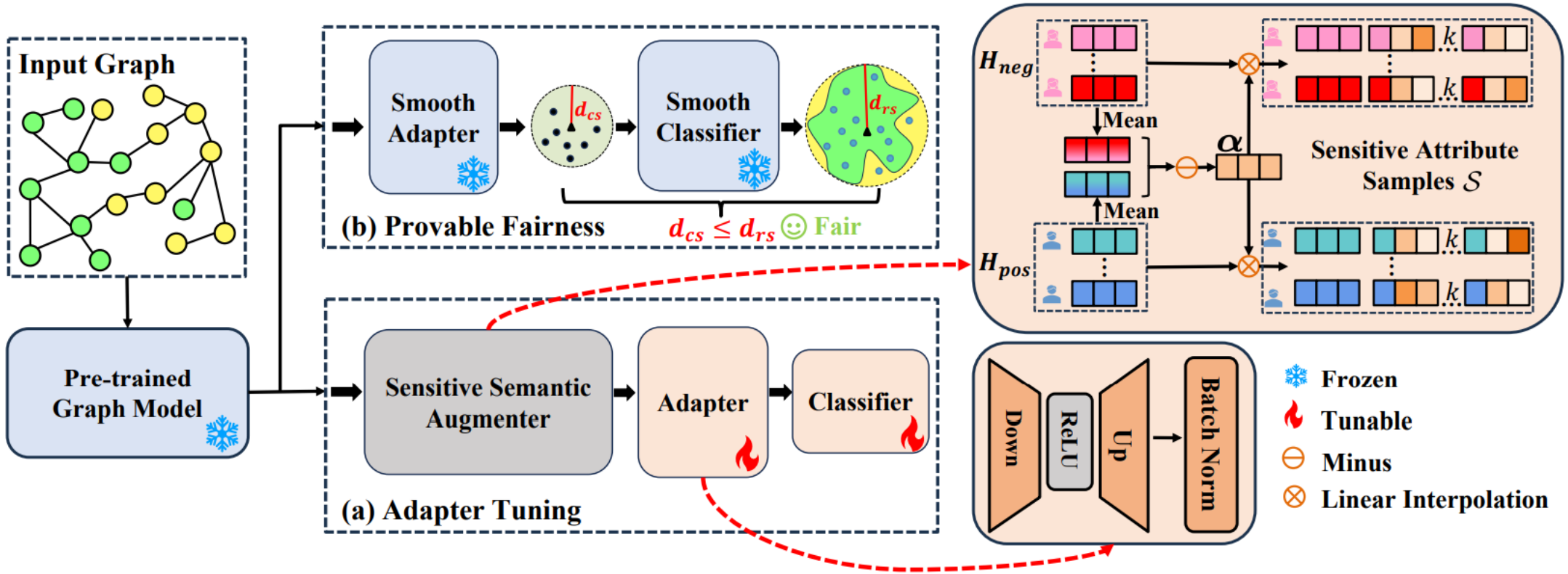
- Existing works generally train a fair GNN for a specific task.
- Debiasing for a specific task in the pre-training phase is inflexible, and maintaining a specific PGM for each task is inefficient.

Existing fair methods lack theoretical guarantees.

- Provable lower bounds on the fairness of model prediction.

How to efficiently and flexibly endow PGMs fairness with practical guarantee?

GraphPAR



Augmenting sensitive attribute semantics

$$\boldsymbol{\alpha} = \mathbf{h}_{pos} - \mathbf{h}_{neg},$$

$$\mathbf{h}_{pos} = \frac{1}{n_{pos}} \sum_{i=1}^{n_{pos}} \mathbf{H}_{pos,i}\,, \mathbf{h}_{neg} = \frac{1}{n_{neg}} \sum_{i=1}^{n_{neg}} \mathbf{H}_{neg,i}$$

$$\mathcal{S}_i := \{\mathbf{h}_i + t \cdot \boldsymbol{\alpha} \mid |t| \leq \epsilon\} \subseteq \mathbb{R}^p,$$

Training adapter for PGMs fairness

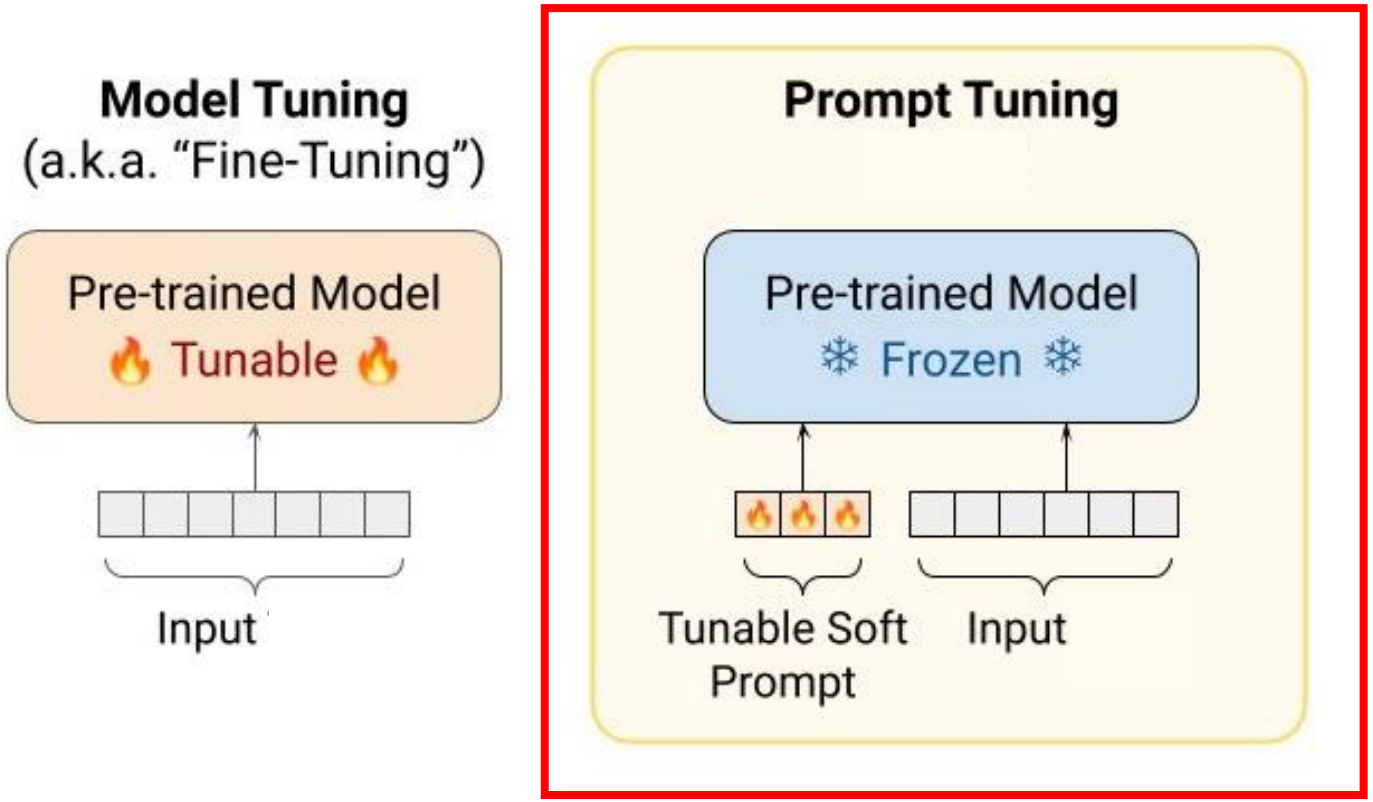
$$\mathcal{L}_{\text{RandAT}} = \mathbb{E}_{i \in \mathcal{V}_L} \left[\mathbb{E}_{\mathbf{h}'_i \in \hat{\mathcal{S}}_i} \left[\ell(d \circ g(\mathbf{h}'_i), y_i) \right] \right],$$

$$\mathcal{L}_{MinMax}\left(\mathbf{h}_i\right) \approx \max_{\mathbf{h}'_i \in \hat{\mathcal{S}}_i} \left\| g\left(\mathbf{h}_i\right) - g\left(\mathbf{h}'_i\right) \right\|_2 .$$

Adaptation

Downstream Adaptation

- Prompt-tuning: keep pre-trained model intact
  - pre-prompt: modify input graph
  - post-prompt: modify output embedding



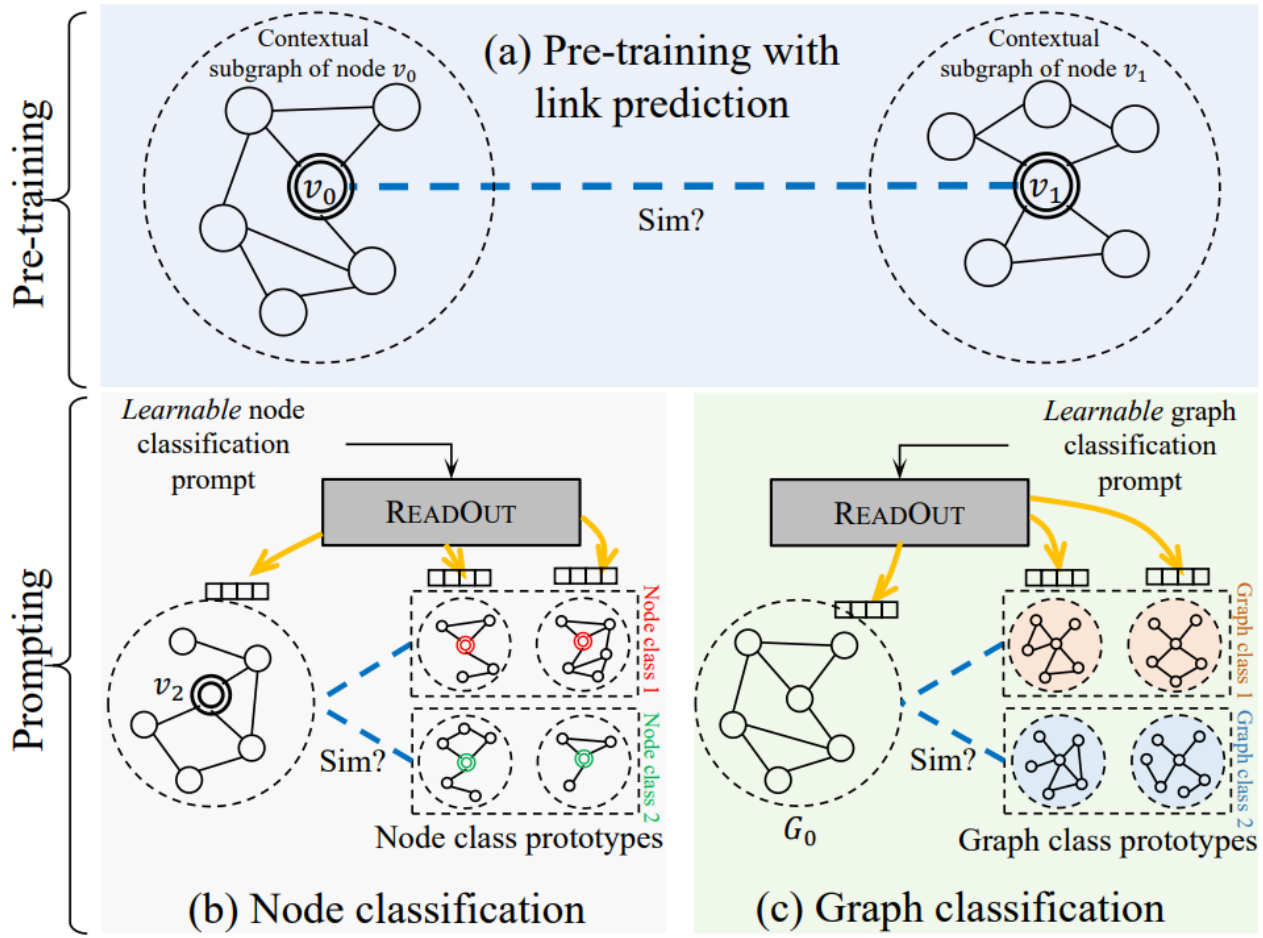
GraphPrompt

Problem:

- How to unify various pre-training and downstream tasks on graph?
- How to design prompts on graph?

Insights：

- A unified task template based on subgraph similarity computation
- Use a learnable prompt to guide graph readout for different tasks



Liu, Z., Yu, X., Fang, Y., & Zhang, X. (2023, April). Graphprompt: Unifying pre-training and downstream tasks for graph neural networks. WWW2023

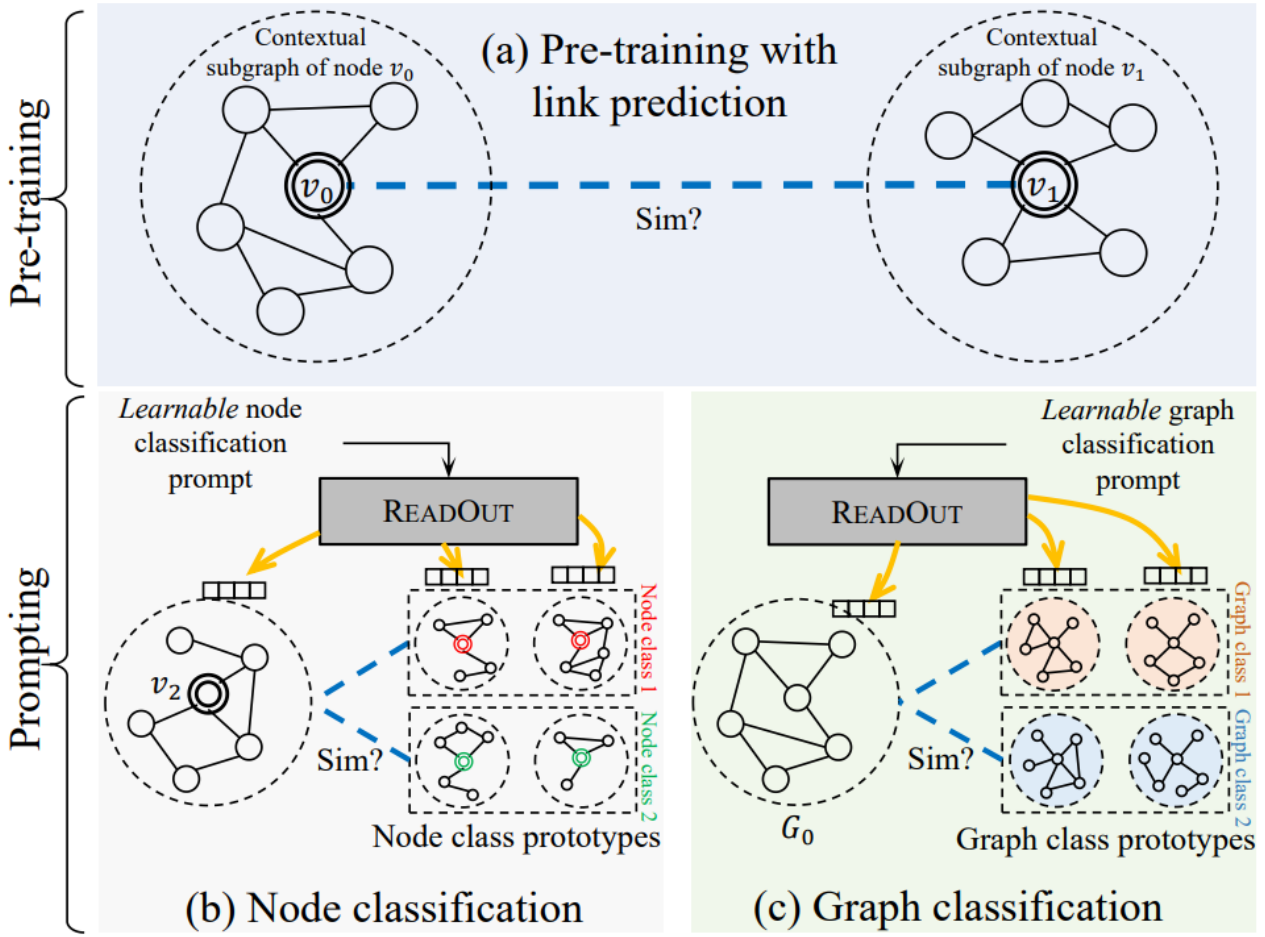
GraphPrompt

Prompt design:

Different downstream tasks require different subgraph readout
→ Use task-specific learnable prompts

Prompt vector added to the readout layer of the pre-trained GNN

$$\mathbf{s}_{t,x} = \textsc{ReadOut}(\{\mathbf{p}_t \odot \mathbf{h}_v : v \in V(S_x)\})$$



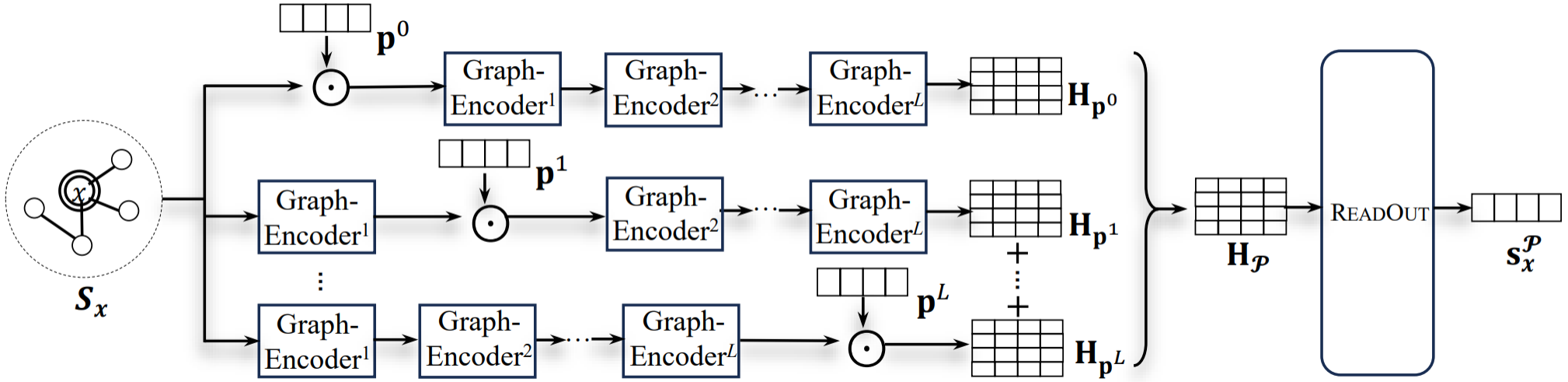
$\mathbf{s}_{t,x}$: (sub)graph embedding of x for a task t
$\mathbf{h}_v$: node v's embedding vector
$\mathbf{p}_t$ or $\mathbf{P}_t$: learnable prompt vector or matrix for task t

Generalized Graph Prompt

Support more pre-training tasks beyond link prediction：

- DGI, InfoGraph, GraphCL, GCC, …

Layer-wise prompts



Yu, X., Liu, Z., Fang, Y., Liu, Z., Chen, S., & Zhang, X. Generalized graph prompt: Toward a unification of pre-training and downstream tasks on graphs. arXiv preprint arXiv:2311.15317.

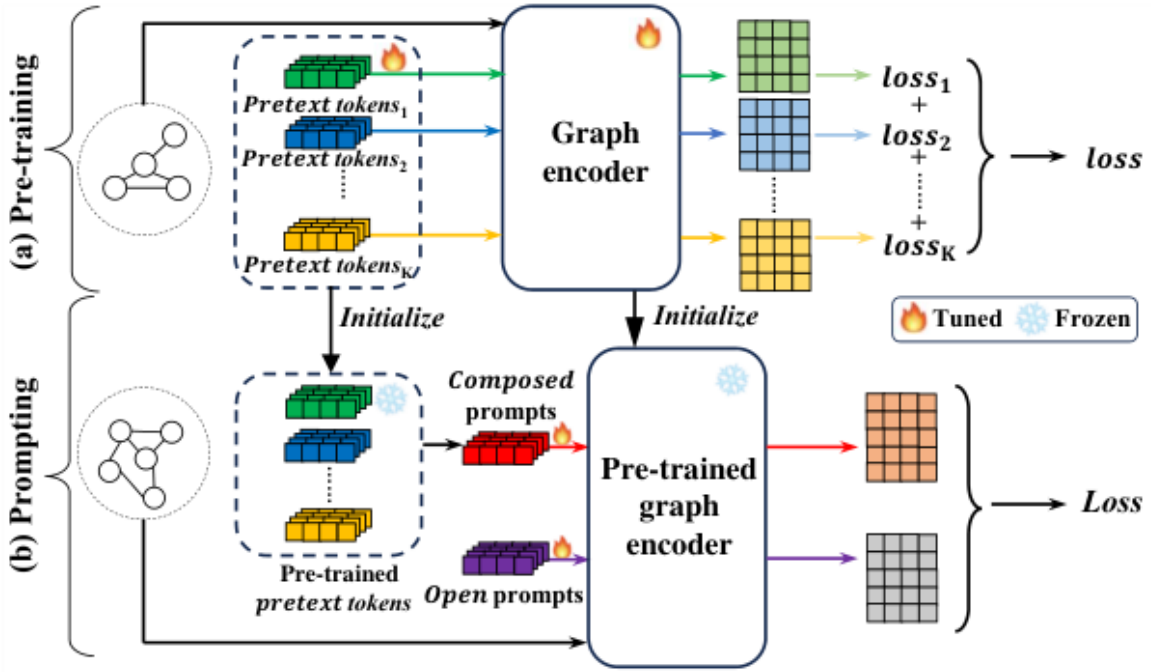
MultiGPrompt

Problem:

- To cater to diverse downstream tasks, pre-training should broadly extract knowledge from various aspects.

Challenges：

- Different pretext tasks often have different objectives, directly combining them lead to task interference.
- Multiple pretext tasks further complicates the alignment of downstream objectives with the pre-trained model.



C1: How can we leverage diverse pre-text tasks for graph models in a synergistic manner?

C2: How can we transfer both task-specific and global pre-trained knowledge

Yu, X., Zhou, C., Fang, Y., & Zhang, X. MultiGPrompt for Multi-Task Pre-Training and Prompting on Graphs. WWW2024

MultiGPrompt

Multi-task pre-training

Pretext tokens

$$\mathcal{T}_{\langle k \rangle} = \{\mathbf{t}_{\langle k \rangle,0}, \mathbf{t}_{\langle k \rangle,1}, \ldots, \mathbf{t}_{\langle k \rangle,L}\}$$

Add token to each layer of graph encoder

$$\mathbf{H}^{l+1} = \mathrm{MP}(\mathbf{t}_{\langle k \rangle,l} \odot \mathbf{H}^{l}, \mathbf{A}; \theta^{l})$$

Graph encoder output embedding

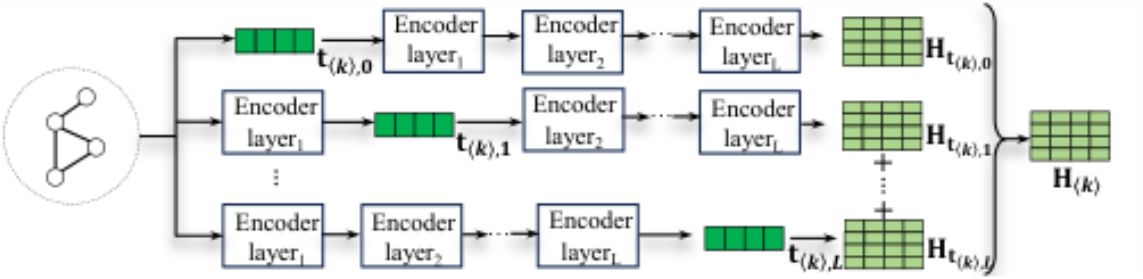
$$\mathbf{H}_{\mathbf{t}} = \textsc{GraphEncoder}_{\mathbf{t}}(\mathbf{X}, \mathbf{A}; \Theta)$$

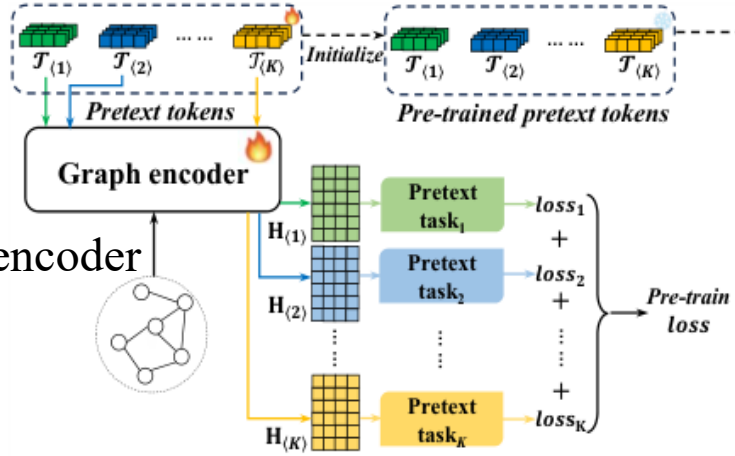
Overall embedding

$$\mathbf{H}_{\langle k \rangle} = \sum_{l=0}^{L} \alpha_l \mathbf{H}_{\mathbf{t}_{\langle k \rangle,l}}$$

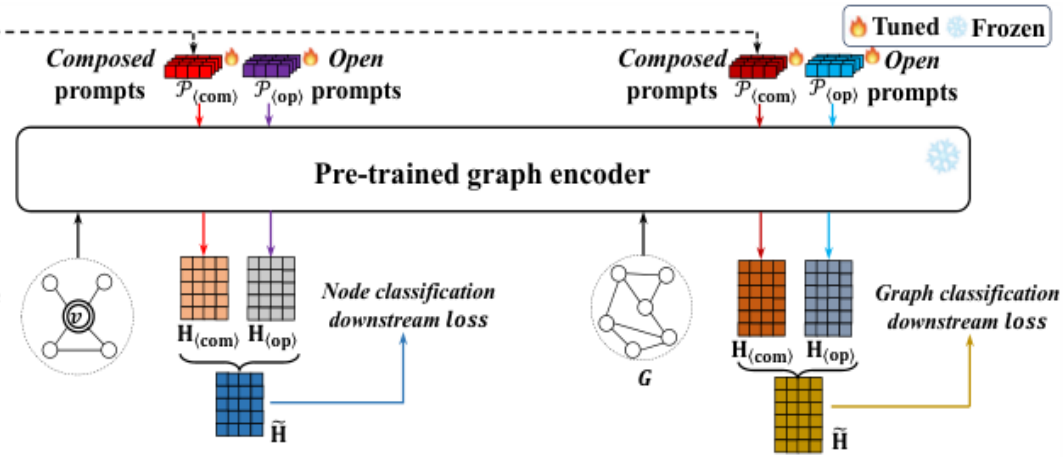
Pre-Training Objective

$$\mathcal{L}_{\mathrm{pre}}(\mathcal{H}; \mathcal{T}, \Theta) = \sum_{k=1}^{K} \beta_k \mathcal{L}_{\mathrm{pre}_{\langle k \rangle}}(\mathbf{H}_{\langle k \rangle}; \mathcal{T}_{\langle k \rangle}, \Theta),$$





(a) Multi-task pre-training



(b) Downstream node classification

(c) Downstream graph classification

Prompt tuning

Composed prompt

$$\mathcal{P}_{\langle \mathrm{com} \rangle} = \{\mathbf{p}_{\langle \mathrm{com} \rangle,0}, \mathbf{p}_{\langle \mathrm{com} \rangle,1}, \ldots, \mathbf{p}_{\langle \mathrm{com} \rangle,L}\}$$

$$\mathbf{p}_{\langle \mathrm{com} \rangle,l} = \textsc{Compose}(\mathbf{t}_{\langle 1 \rangle,l}, \mathbf{t}_{\langle 2 \rangle,l}, \ldots, \mathbf{t}_{\langle K \rangle,l}; \Gamma)$$

Open prompt

$$\mathcal{P}_{\langle \mathrm{op} \rangle} = \{\mathbf{p}_{\langle \mathrm{op} \rangle,0}, \mathbf{p}_{\langle \mathrm{op} \rangle,1}, \ldots, \mathbf{p}_{\langle \mathrm{op} \rangle,L}\}$$

Add prompt to each layer of graph encoder

$$\mathbf{H}_{\mathbf{p}} = \textsc{GraphEncoder}_{\mathbf{p}}(\mathbf{X}, \mathbf{A}; \Theta_{\mathrm{pre}})$$

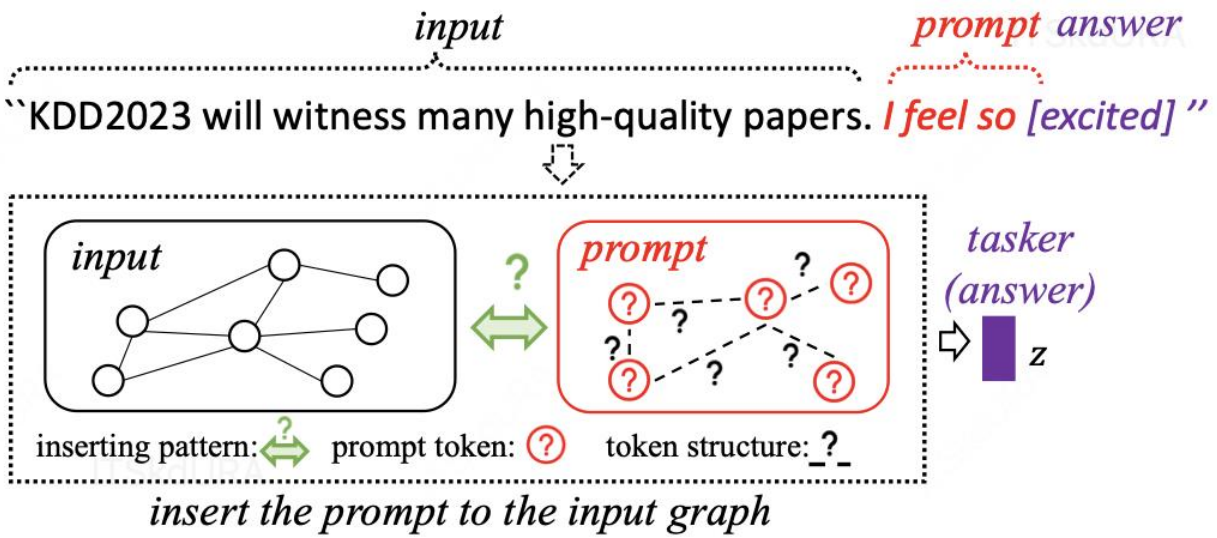
Aggregate dual prompt

$$\tilde{\mathbf{H}} = \textsc{Aggr}(\mathbf{H}_{\langle \mathrm{com} \rangle}, \mathbf{H}_{\langle \mathrm{op} \rangle}; \Delta)$$

All in One

Challenges：

- Graph prompt not only requires the prompt “content” but also needs to know how to organize these tokens and how to insert the prompt into the original graph.
- There is a huge difficulty in reconciling downstream problems to the pre-training task.
- Learning a reliable prompt needs huge manpower and is more sensitive in multi-task setting.

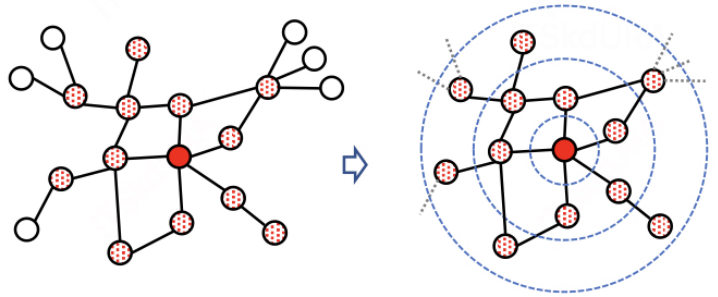


Sun, X., Cheng, H., Li, J., Liu, B., & Guan, J. All in one: Multi-task prompting for graph neural networks. KDD2023

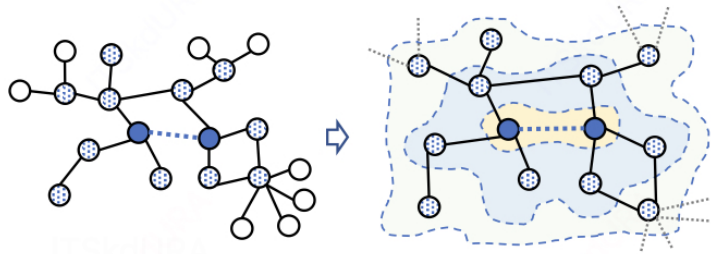
All in One

Reformulate Downstream Tasks：

- This work reformulates node-level and edge-level tasks to graph-level tasks by building induced graphs for nodes and edges, respectively.



(a) Induced graphs for nodes



(b) Induced graphs for edges

Prompt Graph Design：

- This work introduces some prompt nodes with unique connection relationships between them and adaptively insert them into the original input graph, in order to obtain a prompt graph.

HGPrompt: Extending to heterogeneous graphs

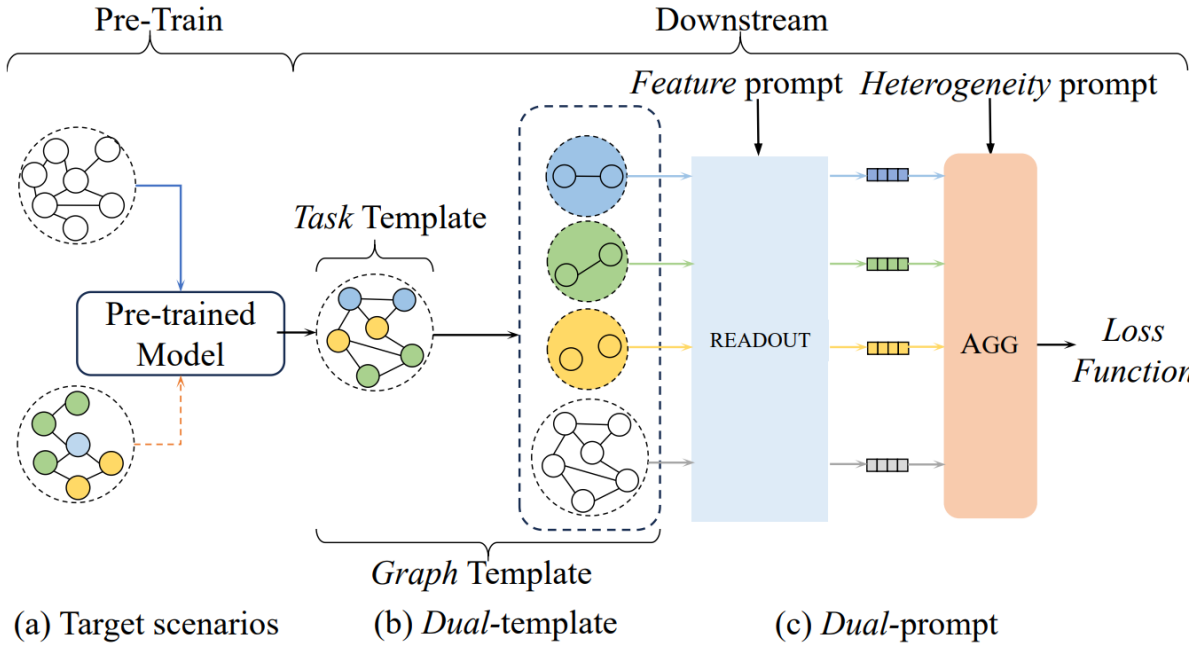
Problem:

- Gap between homogeneous and heterogeneous graph.
- Different downstream tasks focus on heterogeneous aspect.

Insights：

- Dual-template:
  Task + Graph template

- Dual-prompt:
  Feature + Heterogeneity prompt



Yu, X., Fang, Y., Liu, Z., & Zhang, X. Hgprompt: Bridging homogeneous and heterogeneous graphs for few-shot prompt learning. AAAI2024

GPF

Challenges：

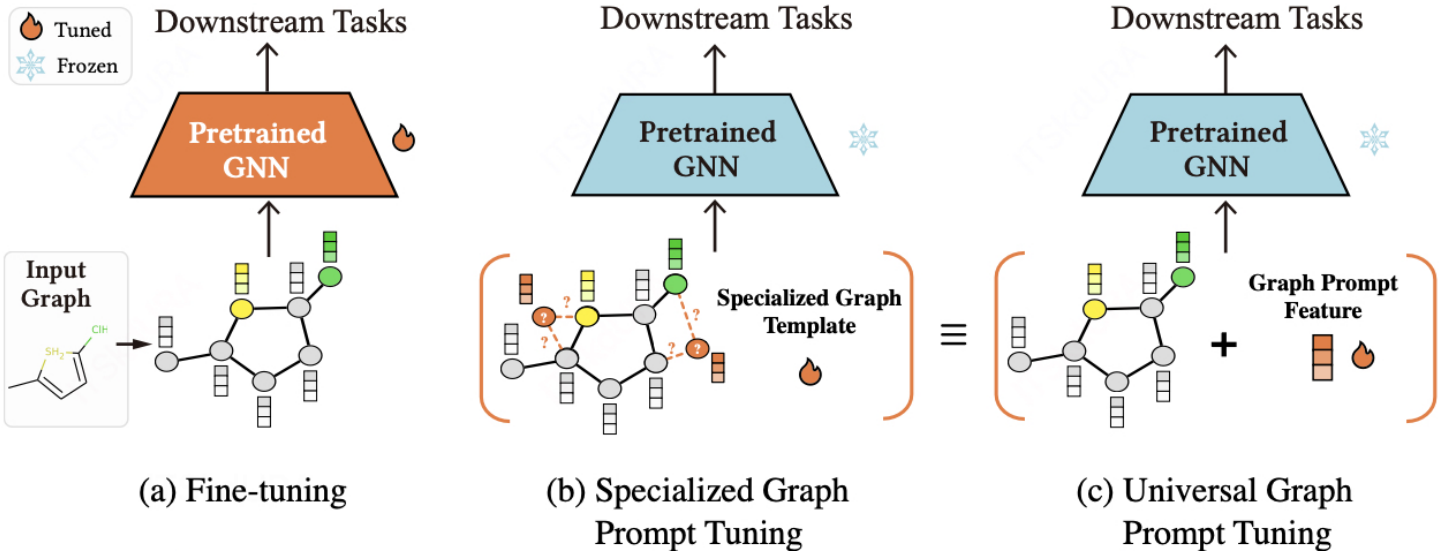
- Diverse pre-training strategies employed on graphs make it difficult to design suitable prompting functions.
- Existing prompt-based tuning methods for GNN models are predominantly designed based on intuition, lacking theoretical guarantees for their effectiveness.

Fang, T., Zhang, Y., Yang, Y., Wang, C., & Chen, L. Universal prompt tuning for graph neural networks. Neurips2023

GPF

Method：

- This work proposes a universal prompt-based tuning method that can be applied to the pre-trained GNN models that employ any pre-training strategy.
- GPF operates on the input graph's feature space and involves adding a shared learnable vector to all node features in the graph.
- GPF-plus is a theoretically stronger variant of GPF, for practical application, which incorporates different prompted features for different nodes in the graph.

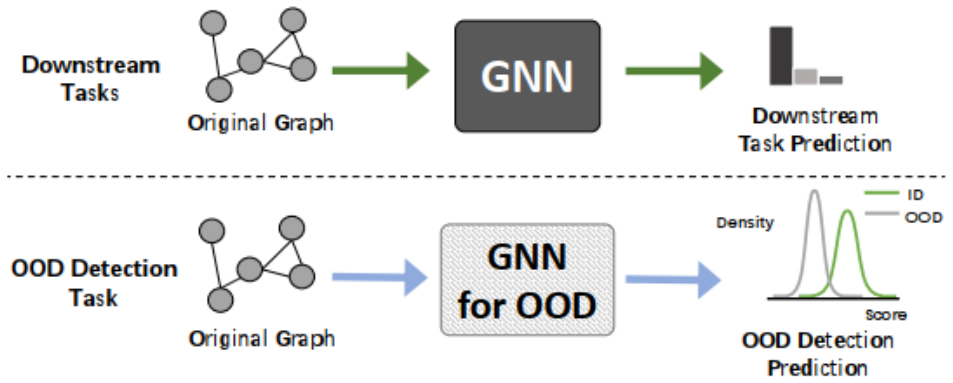


AAGOD

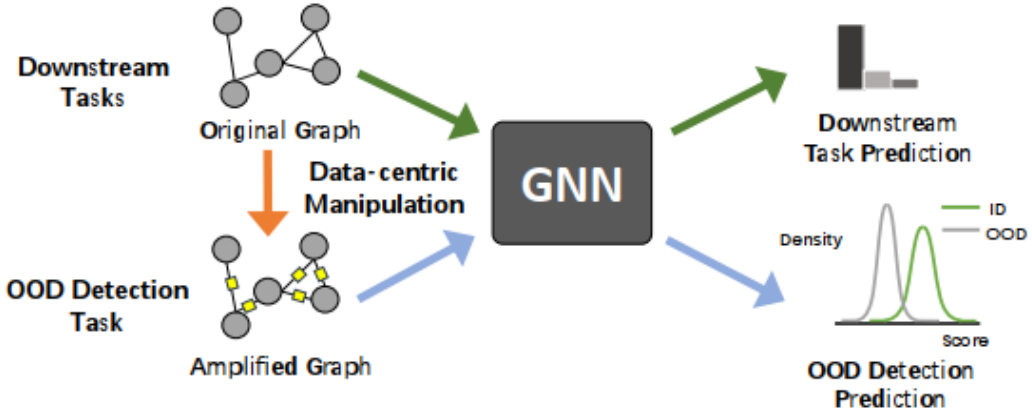
Motivation

- 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

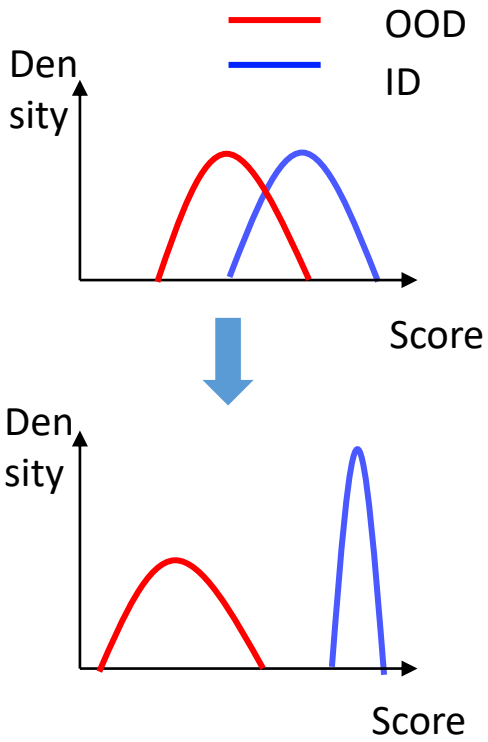


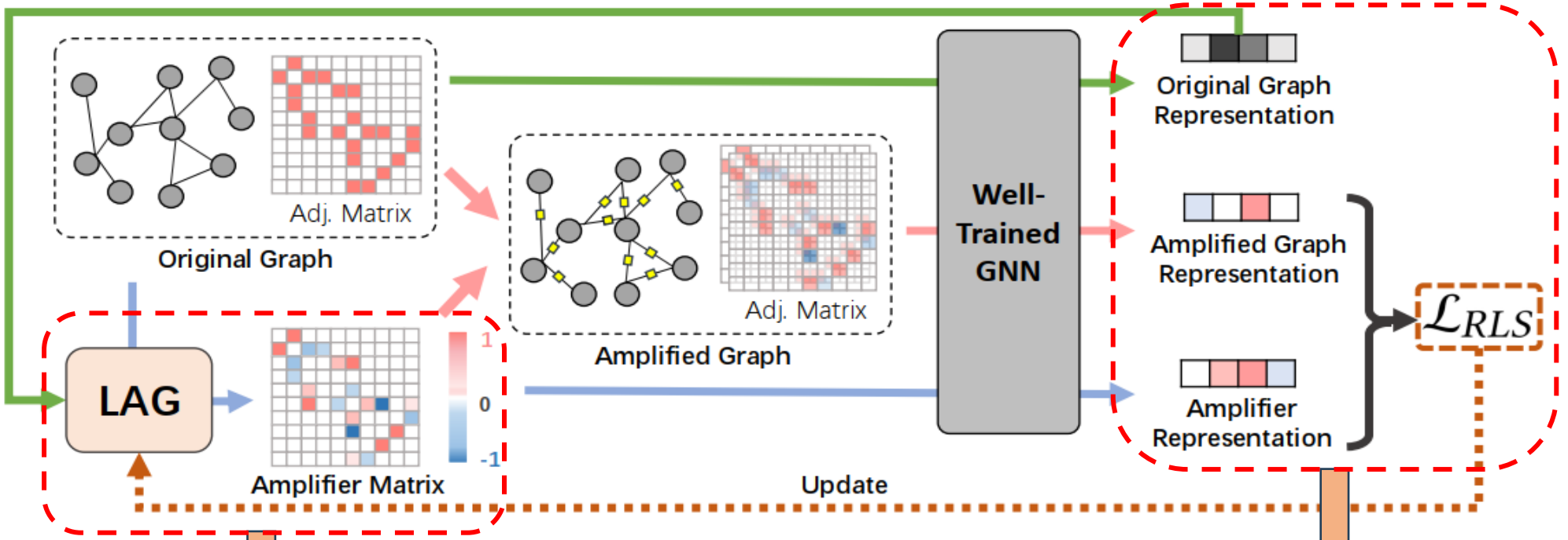
(2) Our proposed framework

Guo, Y., Yang, C., Chen, Y., Liu, J., Shi, C., & Du, J. A Data-centric Framework to Endow Graph Neural Networks with Out-Of-Distribution Detection Ability. KDD2023

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.

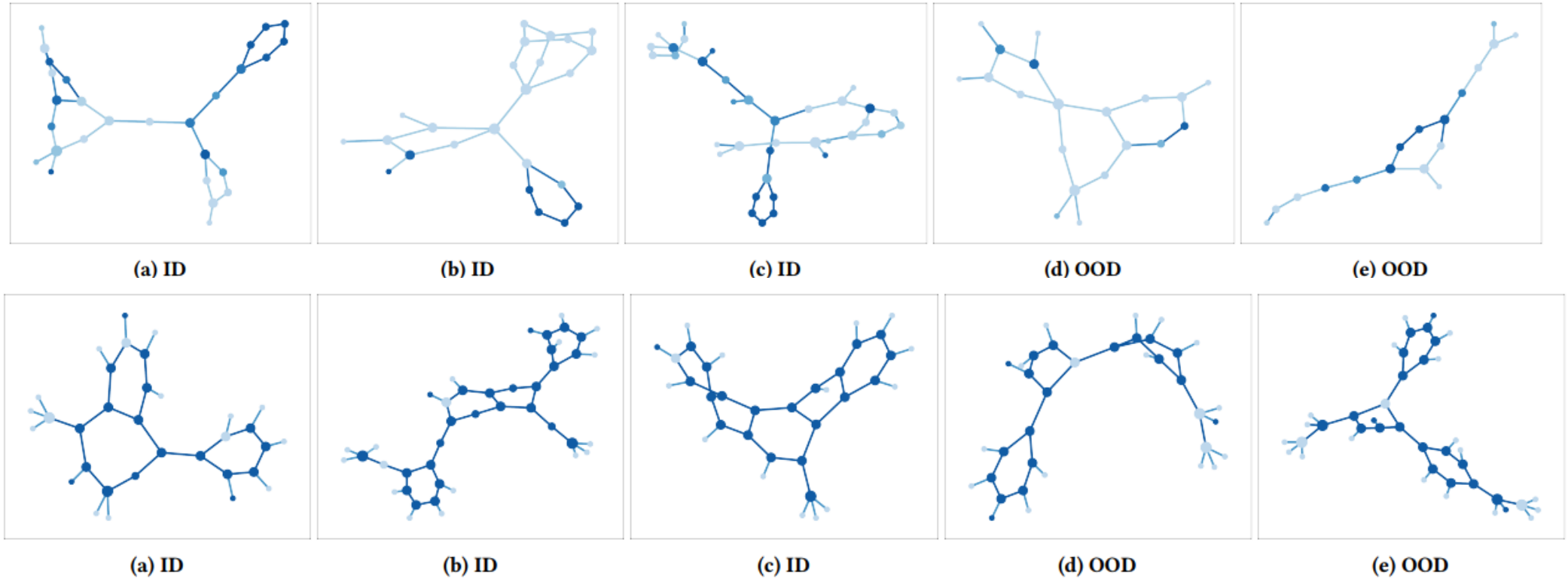
AAGOD

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%

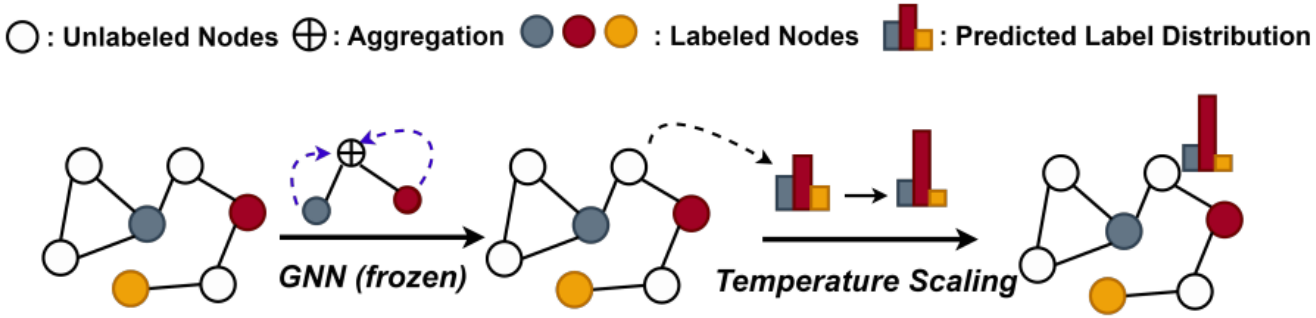
AAGOD

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



DCGC

- Existing calibration methods focus on improving GNN models. Recent work has shown that the post-hoc methods, such as temperature scalling-based calibration, can achieve a better trade-off between accuracy and calibration.



(a) Temperature scaling-based calibration

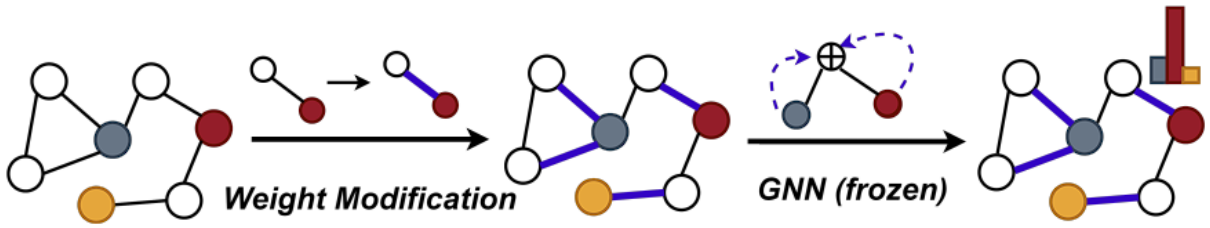
- Through evaluating the expected calibration error (ECE) on Cora and Photo datasets with five different GNNs, we find that the ECEs on Cora (10.25%-18.02%) are always larger than those on Photo (4.38%-8.27%), indicating that **the calibration performance depends more on the datasets instead of GNN model**.

Yang, C., Yang, C., Shi, C., Li, Y., Zhang, Z., & Zhou, J. Calibrating Graph Neural Networks from a Data-centric Perspective. WWW2024

DCGC

- Inspired by this phenomenon, we innovatively propose to calibrate GNNs from a data-centric perspective:

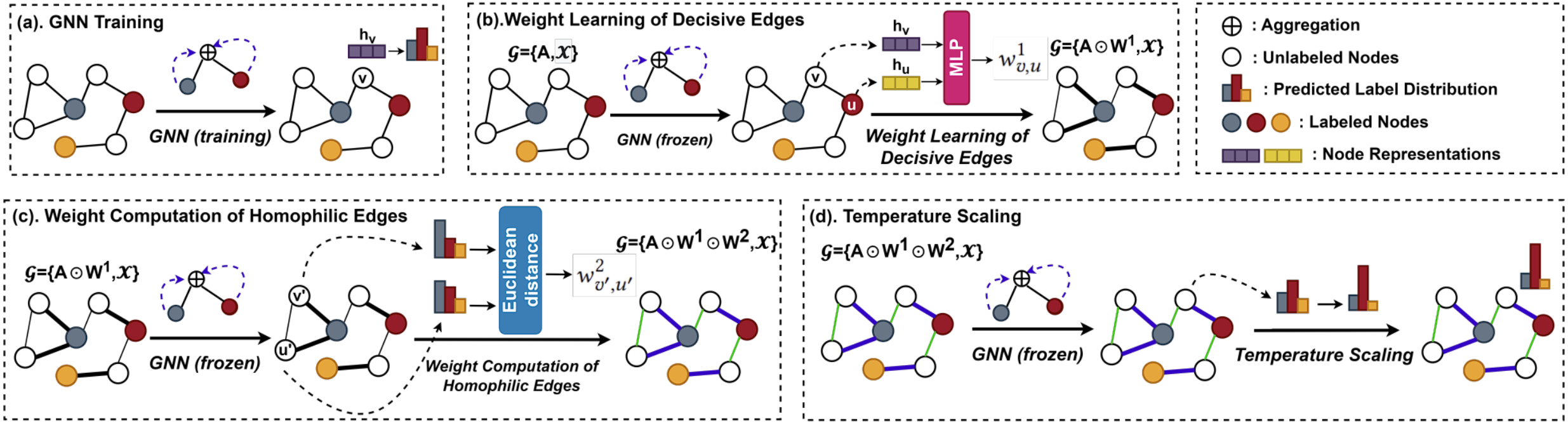
Can we modify the graph data instead for better calibration performance without losing accuracy?



(b) Data-centric calibration

DCGC

- We propose Data-centric Graph Calibration (DCGC) with two edge weighting modules to adjust the input graph.



Summary

GNN-based models compares to foundation models with LLMs

- Advantage：
  - small parameter size, resulting in low-cost training
  - possess essential properties like permutation invariance
  - exhibit strong performance in scenarios without textual attributes
- Disadvantage：
  - limited capacity to harness extensive knowledge and can struggle to manifest emergent abilities
  - underutilize the information stored in textual data

Thanks
Q&A