

EDGE PROMPT TUNING FOR GRAPH NEURAL NETWORKS

Anonymous authors

Paper under double-blind review

ABSTRACT

Pre-training powerful Graph Neural Networks (GNNs) with unlabeled graph data in a self-supervised manner has emerged as a prominent technique in recent years. However, inevitable objective gaps often exist between pre-training and downstream tasks. To bridge this gap, graph prompt tuning techniques design and learn graph prompts by manipulating input graphs or reframing downstream tasks as pre-training tasks without fine-tuning the pre-trained GNN models. While recent graph prompt tuning methods have proven effective in adapting pre-trained GNN models for downstream tasks, they overlook the crucial role of edges in graph prompt design, which can significantly affect the quality of graph representations for downstream tasks. In this study, we propose EdgePrompt, a simple yet effective graph prompt tuning method from the perspective of edges. Unlike previous studies that design prompt vectors on node features, EdgePrompt manipulates input graphs by learning additional prompt vectors for edges and incorporates the edge prompts through message passing in the pre-trained GNN models to better embed graph structural information for downstream tasks. Our method is *compatible* with prevalent GNN architectures pre-trained under various pre-training strategies and is *universal* for different downstream tasks. We provide comprehensive theoretical analyses of our method regarding its capability of handling node classification and graph classification as downstream tasks. Extensive experiments on ten graph datasets under four pre-training strategies demonstrate the superiority of our proposed method against six baselines. Our code is available at <https://anonymous.4open.science/r/EdgePrompt-4905>.

1 INTRODUCTION

Recent years have witnessed the remarkable success of Graph Neural Networks (GNNs) (Kipf & Welling, 2017; Hamilton et al., 2017; Veličković et al., 2018; Xu et al., 2019; Wu et al., 2019; Wang et al., 2019; Chen et al., 2020; Shi & Rajkumar, 2020) for modeling ubiquitous graph-structured data in various real-world scenarios, including social networks (Wei et al., 2023; Zhou et al., 2023), point cloud analysis (Wang et al., 2019; Zhou et al., 2021), and healthcare systems (Cui et al., 2020; Liu et al., 2022b). Such success is mainly attributed to their impressive capability to incorporate node features and graph structures into the representations of graph data. Generally, GNN models are trained for specific downstream tasks in an end-to-end manner. Nevertheless, the end-to-end manner for training powerful GNN models usually encounters significant challenges in practical deployments (Hu et al., 2020b; Sun et al., 2022a; Liu et al., 2023; Fang et al., 2023). First, annotating a sufficient number of labels for graph data is typically time-consuming and resource-intensive in the real world. Second, well-trained GNN models cannot be well generalized to other tasks, even on the same graph data. To grapple with these critical challenges, applying pre-training techniques on graph data has become increasingly prevalent.

Numerous recent studies have focused on designing effective pre-training strategies for training powerful GNN models without using any label information from downstream tasks (Veličković et al., 2019; Hu et al., 2020b; You et al., 2020; Hou et al., 2022; Xia et al., 2022; Xu et al., 2023; Zhang et al., 2023). The philosophy behind these pre-training strategies is to first train a GNN model on pre-training tasks via self-supervised learning and subsequently transfer the pre-trained GNN model to specific downstream tasks. Generally, there exists inevitable objective gaps between pre-training and the downstream tasks. For example, the GNN model can be pre-trained for link

Table 1: A brief comparison of graph prompt tuning methods in the existing studies. (PT=Pre-training, DT=Downstream task)

Method	PT Compatibility	DT Universality	Prompt Insertion
GPPT (Sun et al., 2022a)	✗	✗	Task Embedding
GraphPrompt (Liu et al., 2023)	✓	✓	Readout
GraphPrompt+ (Yu et al., 2024b)	✓	✓	Hidden Representation
ALL-in-one (Sun et al., 2023a)	✓	✓	Node Feature
GPF-plus (Fang et al., 2023)	✓	✓	Node Feature
MultiGPrompt (Yu et al., 2024d)	✗	✓	Hidden Representation
EdgePrompt+ (Ours)	✓	✓	Edge Aggregation

prediction via self-supervised learning, while the downstream task may be node classification. To bridge the objective gap between pre-training and downstream tasks, we typically need to adapt the pre-trained GNN model for downstream tasks by either fine-tuning or graph prompt tuning (Sun et al., 2023b). During fine-tuning, the parameters of the pre-trained GNN model are updated for downstream tasks (Huang et al., 2024; Zhili et al., 2024; Sun et al., 2024). Unlike fine-tuning, graph prompt tuning usually keeps the pre-trained GNN model frozen and instead trains graph prompts for downstream tasks (Sun et al., 2022a; Liu et al., 2023; Fang et al., 2023; Sun et al., 2023a; Tan et al., 2023; Yu et al., 2024b; Ma et al., 2024; Yu et al., 2024a).

While recent graph prompt tuning methods show great prowess in adapting pre-trained GNN models for various downstream tasks (Zi et al., 2024), the existing methods still have several fundamental limitations. First, a few studies (Sun et al., 2022a; Yu et al., 2024d) design graph prompt tuning methods based on specific pre-training strategies, which hinders their application to off-the-shelf pre-trained GNN models. Second, the important dependency information carried by graph structures is ignored in the existing studies (Fang et al., 2023; Liu et al., 2023; Sun et al., 2023a). As illustrated in Table 1, these methods focus on designing and learning graph prompts primarily by applying them to node features or node representations. In this scenario, graph prompts are unable to enhance pre-trained GNN models in capturing complex graph structural information for downstream tasks.

Although the significant role of edges in graph learning has been amplified by a cornucopia of studies (Schlichtkrull et al., 2018; Gong & Cheng, 2019; Vashishth et al., 2020; Jiang et al., 2020; Yang & Li, 2020), unfortunately, none of the existing studies have exploited edges for graph prompt tuning. Naturally, we may ask a question: *how can we devise an edge-level graph prompt tuning method to effectively enhance the performance of a pre-trained GNN model for downstream tasks?* In this study, we aim to answer this question through a pioneering investigation into designing edge prompts for downstream tasks. In our investigation, we need to overcome two key challenges. First, edge prompt design needs to be *universal*, capable of handling graphs of varying sizes and different downstream tasks, such as node classification and graph classification. Second, edge prompt design must be *compatible* with prevalent GNN models pre-trained by various strategies, especially with those that cannot accommodate edge attributes. These two challenges make the edge prompt design nontrivial, requiring an ingenious approach to graph prompt tuning.

To address the above issues, we propose a novel graph prompt tuning method named EdgePrompt purely from the perspective of edges, fundamentally differing from node-level prompt designs in the existing studies (Sun et al., 2023a; Fang et al., 2023). The intuition of EdgePrompt is to manipulate the input graph by adding extra learnable prompt vectors to edges and thereby enhance the capability of pre-trained GNN models for downstream tasks. In EdgePrompt, all the edges in the input graph learn a shared prompt vector at each layer of the pre-trained GNN model. The edge prompts will be aggregated along with node representations during the forward pass of the message-passing mechanism. To further enhance the capacity of edge prompts, we propose an advanced version EdgePrompt+ that enables each edge to learn its customized prompt vectors. We provide theoretical analyses to support that our proposed method has the capability of enhancing the pre-trained GNN models for downstream tasks. We conduct extensive experiments over ten graph datasets under four pre-training strategies. The results validate the superiority of our proposed method compared with six baselines. Our contributions to this study can be summarized as follows:

- We devise a simple yet effective graph prompt tuning method, EdgePrompt and its variant EdgePrompt+, from the perspective of edges to narrow the objective gap between pre-training and downstream tasks.
- We provide comprehensive analyses of our method regarding its capability of handling various downstream tasks, including node classification and graph classification.
- We conduct extensive experiments over ten datasets under four pre-training strategies to evaluate the effectiveness of our proposed method. Experimental results demonstrate the superiority of our method compared with six baselines for both node classification and graph classification tasks.

2 RELATED WORK

Graph Pre-training. Numerous studies have proposed to train powerful GNN models via self-supervised learning (Veličković et al., 2019; Sun et al., 2020; Hu et al., 2019; You et al., 2020; Jin et al., 2020; Rossi et al., 2020; Xia et al., 2022; Hou et al., 2022; Xu et al., 2023; Zhang et al., 2023). These studies can be roughly categorized into two genres: contrastive methods and generative methods. Contrastive methods typically aim to maximize the agreement between augmented instances of the same object. For instance, DGI (Veličković et al., 2019) and InfoGraph (Sun et al., 2020) adopt the mutual information maximization between the local augmented instances and the global representation. GraphCL (You et al., 2020) maximizes the agreement between two views of the same graph by different augmentation strategies. SimGRACE (Xia et al., 2022) uses GNN models with perturbed parameters to obtain contrastive views without data augmentation. In the meantime, generative methods attempt to pre-train GNN models by reconstructing specific information in the input graph. For example, GraphMAE (Hou et al., 2022) pre-trains GNNs by reconstructing masked node features. In addition, edge prediction is also employed as the pre-training technique by a cornucopia of studies (Rossi et al., 2020; Jin et al., 2020; Sun et al., 2022a; Liu et al., 2023).

Graph Prompt Tuning. To bridge the gap between pre-training and downstream tasks, graph prompt tuning methods modify the input graph with learnable prompt vectors for downstream tasks, while keeping the pre-trained GNN model frozen. For example, GPF-plus (Fang et al., 2023) transforms the input graph to a prompted one by adding extra learnable prompt vectors to node features for downstream tasks. All-in-one (Sun et al., 2023a) unifies various downstream tasks as graph-level tasks and similarly learns prompt vectors that are added to node features. GPPT (Sun et al., 2022a) mainly focuses on node classification as the downstream task and adopts link prediction as the pre-training strategy. It narrows the gap between pre-training and downstream tasks by converting node classification to link prediction. GraphPrompt (Liu et al., 2023) designs graph prompts as a feature weighting vector to obtain task-specific (sub)graph-level representations. MultiGPrompt (Yu et al., 2024d) chooses to insert prompt vectors into node representations at each hidden layer. However, all the aforementioned studies ignore the role of edges when designing graph prompts, which are widely regarded as fundamental properties in graph data.

3 PRELIMINARIES

3.1 GRAPH NEURAL NETWORKS

Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ denote a graph where $\mathcal{V} = \{v_1, v_2, \dots, v_N\}$ is the set of N nodes, and \mathcal{E} is the edge set. $\mathbf{X} \in \mathbb{R}^{N \times D}$ denotes the node feature matrix where the i -th row \mathbf{x}_i represents a D -dimensional feature vector of node $v_i \in \mathcal{V}$. The edges in \mathcal{G} can also be represented by an adjacency matrix $\mathbf{A} \in \{0, 1\}^{N \times N}$ where each entry $a_{ij} = 1$ if $(v_i, v_j) \in \mathcal{E}$, otherwise $a_{ij} = 0$. Generally, GNN models aim to learn expressive node representations through the message-passing mechanism (Kipf & Welling, 2017; Veličković et al., 2018; Hamilton et al., 2017; Xu et al., 2019) where the representation of a target node is iteratively updated by aggregating the representations of its neighboring nodes. Specifically, a GNN model has two fundamental operators: $\text{AGG}(\cdot)$ extracting the neighboring information of the node, and $\text{COMB}(\cdot)$ integrating the previous representation of the node and its neighboring information. Mathematically, the l -th layer of an L -layer GNN model f updates the representation of node $v_i \in \mathcal{V}$ by

$$\mathbf{h}_i^{(l)} = \text{COMB}^{(l)}(\mathbf{h}_i^{(l-1)}, \text{AGG}^{(l)}(\{\mathbf{h}_j^{(l-1)} : v_j \in \mathcal{N}(v_i)\})), \quad (1)$$

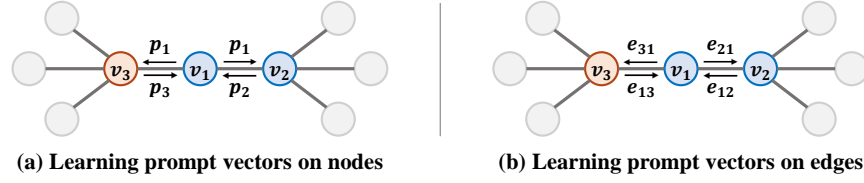


Figure 1: Learning prompt vectors on a node may uniformly pass them to its neighboring nodes while learning prompt vectors on edges can result in customized prompt aggregation.

where $\mathbf{h}_i^{(l)} \in \mathbb{R}^{D_l}$ denotes the D_l -dimensional representation of node v_i at the l -th layer, and $\mathcal{N}(v_i)$ denotes the neighbors of node v_i . $\mathbf{h}_i^{(0)} \in \mathbb{R}^D$ is initialized with node v_i 's feature \mathbf{x}_i . The final node representation $\mathbf{h}_i^{(L)}$ after the L -th layer of the GNN model can be subsequently used for various downstream tasks (e.g., node classification and graph classification) with a trainable classifier g .

4 METHODOLOGY

In this section, we present our proposed method EdgePrompt and its variant EdgePrompt+. Figure 1 illustrates the difference between node prompt-based methods (Sun et al., 2023a; Fang et al., 2023) and our edge prompt-based method. We first formulate the research problem studied in this paper. Then we introduce our design on edge prompts in EdgePrompt and EdgePrompt+ in detail. Furthermore, we provide comprehensive analyses to demonstrate that our method has the capability of benefiting pre-trained GNN models for node classification tasks. At last, we extend our method to graph classification as the downstream task.

4.1 PROBLEM SETTING

This study focuses on the standard problem of graph prompt tuning following previous studies (Fang et al., 2023; Sun et al., 2023a). We consider a GNN model pre-trained by a pre-training task. We aim to adapt the pre-trained GNN model to a downstream task on a graph dataset through graph prompt tuning while keeping its parameters frozen. Specifically, given a pre-trained GNN model f , the goal is to transform the input graph \mathcal{G} to a prompted graph $\mathcal{G}' = \mathcal{T}(\mathcal{G})$ with learnable prompts and obtain expressive node representations on \mathcal{G}' by f for a specific downstream task. Here, \mathcal{T} is a graph transformation to obtain \mathcal{G}' by adding prompts to \mathcal{G} . The key problem in graph prompt tuning is to design and learn suitable graph prompts to benefit downstream tasks.

4.2 EDGE PROMPT DESIGN

Inspired by pixel-level visual prompts (Bahng et al., 2022; Wu et al., 2022) in Computer Vision, the existing studies (Sun et al., 2023a; Fang et al., 2023) design graph prompts at the data level by adding extra learnable prompt vectors to node features. Nevertheless, this strategy does not take account of the dependencies between nodes in graph data, which can significantly impact the final node representations via the message-passing mechanism in GNN models (Fatemi et al., 2021; Sun et al., 2022b; Liu et al., 2022a;c). Motivated by this, we propose to design our graph prompt tuning method from the perspective of edges in this study.

EdgePrompt. Considering the dependencies between nodes in graph data, we design learnable prompt vectors on edges and manipulate the input graph to a prompted one with the edge prompts; therefore, the pre-trained GNN model can generate expressive node representations on the prompted graph for the downstream task. More concretely, for each edge $(v_i, v_j) \in \mathcal{E}$, we aim to learn a prompt vector $\mathbf{e}_{ij}^{(l)} \in \mathbb{R}^{D_{l-1}}$ on it at the l -th layer of the pre-trained GNN model. Typically, this prompt vector can be regarded as the learnable properties of edges. As discussed previously, one critical challenge arises here: many popular GNN models, such as GCN (Kipf & Welling, 2017), do not accommodate edge attributes during the message-passing mechanism. Therefore, they are unable to absorb $\mathbf{e}_{ij}^{(l)}$ into node representations. To overcome this issue, we propose to aggregate the prompt vector along with node representations through the message-passing mechanism during

the forward pass at each layer of the pre-trained GNN model. Specifically, to compute $\mathbf{h}_i^{(l)}$ of each node v_i at the l -th layer, the GNN model will aggregate not only $\mathbf{h}_j^{(l-1)}$ from its neighboring node $v_j \in \mathcal{N}(v_i)$ but also $\mathbf{e}_{ij}^{(l)}$ associated with edge (v_i, v_j) . Mathematically, we can reformulate Equation (1) with the edge prompt vector at the l -th layer of the pre-trained GNN model by

$$\mathbf{h}_i^{(l)} = \text{COMB}^{(l)}(\mathbf{h}_i^{(l-1)}, \text{AGG}^{(l)}(\{\mathbf{h}_j^{(l-1)} : v_j \in \mathcal{N}(v_i)\}, \{\mathbf{e}_{ij}^{(l)} : v_j \in \mathcal{N}(v_i)\})). \quad (2)$$

To obtain the prompt vector, one simple yet effective way is to learn a global prompt vector shared by all the edges. Let $\mathbf{p}^{(l)} \in \mathbb{R}^{D_{l-1}}$ denote the global prompt vector at the l -th layer of the pre-trained GNN model. The prompt vector for each edge (v_i, v_j) at the l -th layer can be written as

$$\mathbf{e}_{ij}^{(l)} = \mathbf{p}^{(l)}, \quad \forall (v_i, v_j) \in \mathcal{E}. \quad (3)$$

The above design with global prompt vectors on edges is termed EdgePrompt in our method.

EdgePrompt+. Although EdgePrompt designs graph prompts from the perspective of edges, a single shared prompt vector for all the edges is insufficient to model different complex dependencies between nodes. Motivated by this, we conceive an advanced version of the above EdgePrompt, called EdgePrompt+, to learn customized prompt vectors on edges. Specifically, instead of using a shared prompt vector $\mathbf{p}^{(l)}$ for all the edges at the l -th layer, each edge $(v_i, v_j) \in \mathcal{E}$ will learn its own customized prompt vector $\mathbf{e}_{ij}^{(l)}$. Nevertheless, learning $|\mathcal{E}|$ independent prompt vectors is infeasible in practice. When we optimize prompt vectors for downstream tasks (e.g., node classification), we may have only a limited number of labeled nodes. Therefore, most edges cannot receive supervision information (Fatemi et al., 2021) for optimizing their prompt vectors, especially in a few-shot setting (Zi et al., 2024). In this case, it will be hard to directly learn $\mathbf{e}_{ij}^{(l)}$ for edge $(v_i, v_j) \in \mathcal{E}$ if it is not involved in computing the representations of any labeled nodes. To overcome this issue, we propose to learn the prompt vectors as a weighted average of multiple anchor prompts. To achieve this, we first construct a set of M_l anchor prompts $\mathcal{P}^{(l)} = \{\mathbf{p}_1^{(l)}, \mathbf{p}_2^{(l)}, \dots, \mathbf{p}_{M_l}^{(l)}\}$ at the l -th layer of the pre-trained GNN model, where each vector $\mathbf{p}_m^{(l)} \in \mathbb{R}^{D_{l-1}}$ is a learnable anchor prompt. For each edge $(v_i, v_j) \in \mathcal{E}$, its customized prompt vector $\mathbf{e}_{ij}^{(l)}$ at the l -th layer is computed as the weighted average of the anchor prompts in $\mathcal{P}^{(l)}$ with the score vector $\mathbf{b}_{ij}^{(l)} \in \mathbb{R}^{M_l}$. Mathematically, we can obtain $\mathbf{e}_{ij}^{(l)}$ at the l -th layer by

$$\mathbf{e}_{ij}^{(l)} = \sum_{m=1}^{M_l} \mathbf{b}_{ijm}^{(l)} \cdot \mathbf{p}_m^{(l)}, \quad (4)$$

where $\mathbf{b}_{ijm}^{(l)}$ denotes the m -th entry in $\mathbf{b}_{ij}^{(l)}$. Since all the edges share the same anchor prompts $\mathcal{P}^{(l)}$ at the l -th layer, the score vector $\mathbf{b}_{ij}^{(l)}$ directly determines how $\mathbf{e}_{ij}^{(l)}$ differs from those of the other edges. Therefore, our next goal is to conceive an effective strategy to obtain the desired $\mathbf{b}_{ij}^{(l)}$. According to Equation (2), $\mathbf{e}_{ij}^{(l)}$ of edge (v_i, v_j) affects message passing between nodes v_i and v_j , so we may naturally consider $\mathbf{b}_{ij}^{(l)}$ to depend on both nodes v_i and v_j . Motivated by this, we propose to compute $\mathbf{b}_{ij}^{(l)}$ at the l -th layer using a score function $\phi^{(l)}$ followed by the softmax operation. Formally, we compute $\mathbf{b}_{ij}^{(l)}$ by

$$\mathbf{b}_{ij}^{(l)} = \text{Softmax}(\phi^{(l)}(v_i, v_j)), \quad (5)$$

where $\text{Softmax}(\cdot)$ represents the softmax operation. Here, $\phi^{(l)}$ takes each pair of nodes v_i and v_j as the input and generates the score vector. Basically, it describes the relationship of two nodes at the l -th layer and embeds them into a single vector. Many typical formulations (Veličković et al., 2018; Brody et al., 2022; Yang et al., 2021) can be used to achieve this goal. In this study, we adopt the classic attention mechanism (Veličković et al., 2018) as $\phi^{(l)}$ by

$$\phi^{(l)}(v_i, v_j) = \text{LeakyReLU}([\mathbf{h}_i^{(l-1)} \parallel \mathbf{h}_j^{(l-1)}] \cdot \mathbf{W}^{(l)}), \quad (6)$$

where $\mathbf{W}^{(l)} \in \mathbb{R}^{2D_{l-1} \times M_l}$ is the weight matrix of $\phi^{(l)}$ at the l -th layer, and $[\cdot \parallel \cdot]$ denotes the vector concatenation. In-depth investigations into different variants of the score function ϕ will be reserved

for our future work. It is worth noting that GPF-plus (Fang et al., 2023) can be regarded as a special case of EdgePrompt+ with the score function as a linear mapping of x_i .

With the learnable edge prompts, we can obtain more suitable node representations $h_i^{(L)}$ for node $v_i \in \mathcal{V}$ by the pre-trained GNN model for node classification. Given the labeled node set $\mathcal{V}_L \in \mathcal{V}$, we optimize our edge prompts and a classifier g by

$$\min_{g, \{\mathcal{P}^{(1)}, \dots, \mathcal{P}^{(L)}, \mathbf{W}^{(1)}, \dots, \mathbf{W}^{(L)}\}} \frac{1}{|\mathcal{V}_L|} \sum_{v_i \in \mathcal{V}_L} \ell_D(g(f(\mathcal{G}')_i), y_i), \quad (7)$$

where y_i is the ground-truth label of node $v_i \in \mathcal{V}_L$, and ℓ_D is the downstream task loss, i.e., the cross-entropy loss for classification tasks.

4.3 ANALYSIS OF EDGE PROMPT TUNING FOR NODE CLASSIFICATION

In this subsection, we provide a comprehensive analysis to investigate why our proposed EdgePrompt+ is more effective for node classification than existing approaches, particularly those that focus on learning additional prompt vectors on node features.

We first provide our insights regarding the issue of uniform message passing on prompt vectors. As introduced previously, GPF-plus (Fang et al., 2023) and All-in-one (Sun et al., 2023a) design learnable prompt vectors on the node level and manipulate the input graph by adding the prompt vectors to node features. For each node v_i , its learned prompt vector p_i completely depends on its node feature x_i . In many prevalent GNN models, such as GCNs, the prompt vector will be uniformly aggregated by neighboring nodes through the message-passing mechanism (Yang et al., 2021). Taking node v_1 in Figure 1(a) as an example, its two neighboring nodes v_2 and v_3 will always receive the same prompt vector p_1 from node v_1 in pre-trained GCN models. Unfortunately, such propagation of prompt vectors may not benefit node classification. Instead, the prompt vector aggregated by a node can retain adverse information from different classes. In contrast, our proposed EdgePrompt+ designs prompt vectors on edges. Unlike one shared prompt vector of a node for all its neighboring nodes, EdgePrompt+ enables these neighboring nodes to receive different learned prompt vectors (e.g., e_{21} and e_{31} in Figure 1(b)) from the node. In this way, the issue of uniform passing on prompt vectors can be mitigated.

Furthermore, we would like to provide a theoretical analysis of how edge prompts in our proposed EdgePrompt+ can benefit node classification. Our analysis is based on random graphs generated by the contextual stochastic block model (CSBM) (Tsitsulin et al., 2022; Ma et al., 2022). Specifically, we consider a random graph \mathcal{G} generated by the CSBM consisting of two node classes c_1 and c_2 . For each node v_i , its node feature x_i follows a Gaussian distribution $x_i \sim \mathcal{N}(\mu_1, \mathbf{I})$ if it is from class c_1 , otherwise $x_i \sim \mathcal{N}(\mu_2, \mathbf{I})$. Generally, we assume $\mu_1 \neq \mu_2$. In the graph \mathcal{G} , edges are generated following an intra-class probability p and an inter-class probability q . More concretely, a pair of nodes will be connected by an edge with probability p if they are from the same class; otherwise, the probability is q . In this section, we use $\mathcal{G} \sim \text{CSBM}(\mu_1, \mu_2, p, q)$ to denote a random graph generated by the CSBM.

Our analysis aims to investigate the improvement of linear separability under pre-trained GCN models caused by edge prompts in EdgePrompt+. Specifically, we focus on the linear classifiers with the largest margin based on node representations after GCN operations with and without edge prompts. Typically, if the expected distance between the two class centroids is larger, the node representations will have higher linear separability by the linear classifier.

Theorem 1. *Given a random graph $\mathcal{G} \sim \text{CSBM}(\mu_1, \mu_2, p, q)$ and a pre-trained GCN model f , there always exist a set of $M \geq 2$ anchor prompts $\mathcal{P} = \{p_1, p_2, \dots, p_M\}$ and the score vectors $b_{i,j}$ for each edge (v_i, v_j) that improve the expected distance after GCN operation between classes c_1 and c_2 to T times without using edge prompts, where $T \in (1, 1 + \frac{p}{|p-q|}]$.*

A detailed proof can be found in Appendix A. According to Theorem 1, we will have a larger expected distance between the two class centroids after GCN operation with edge prompts in EdgePrompt+. In this case, the node representations from the two classes will have a lower probability of being misclassified. Therefore, we can conclude that our proposed EdgePrompt+ benefits pre-trained GNN models for node classification.

4.4 EXTENSION TO GRAPH CLASSIFICATION

In the last subsection, we present our edge prompt design in EdgePrompt and EdgePrompt+ for node classification. As discussed previously, edge prompts should be capable of handling various downstream tasks, including graph classification. In this subsection, we would like to introduce how EdgePrompt and EdgePrompt+ tackle graph classification.

In graph classification, we have a set of labeled graphs $\{\mathcal{G}_1, \mathcal{G}_2, \dots, \mathcal{G}_K\}$ with their label set $\{y_1, y_2, \dots, y_K\}$. To obtain the representation of the entire graph \mathcal{G} , we typically integrate the final representations of all nodes in \mathcal{G} via a permutation-invariant READOUT function (Xu et al., 2019), such as *sum* and *mean*, as the entire graph’s representation $\mathbf{h}_{\mathcal{G}} = \text{READOUT}(\{\mathbf{h}_i | v_i \in \mathcal{V}\})$. Therefore, we can optimize our edge prompts and a classifier g by

$$\min_{g, \{\mathcal{P}^{(1)}, \dots, \mathcal{P}^{(L)}, \mathbf{W}^{(1)}, \dots, \mathbf{W}^{(L)}\}} \frac{1}{K} \sum_{k=1}^K \ell_D(g(f(\mathcal{G}'_k)), y_k). \quad (8)$$

Now we analyze the capability of EdgePrompt for graph classifications. The goal of our analysis is to investigate whether learning edge prompts in EdgePrompt can result in consistent graph representations with those using any prompt strategies. To this end, we propose the following theorem.

Theorem 2. *Given an input graph $\mathcal{G} = (\mathbf{X}, \mathbf{A})$ and its transformation $\mathcal{G}' = (\mathbf{X}', \mathbf{A}')$ by an arbitrary transformation function \mathcal{T} , there exists a set of edge prompt vectors $\{\mathbf{p}^{(1)}, \mathbf{p}^{(2)}, \dots, \mathbf{p}^{(L)}\}$ in EdgePrompt that can satisfy*

$$f(\mathbf{X}, \mathbf{A}, \{\mathbf{p}^{(1)}, \dots, \mathbf{p}^{(L)}\}) = f(\mathbf{X}', \mathbf{A}') \quad (9)$$

for any pre-trained GNN model f .

The complete proof of Theorem 2 is provided in Appendix B. According to Theorem 2, we can conclude that our edge prompts have the capability to get graph \mathcal{G} ’s representation which is equal to those of its variants by transformations with any prompt strategies. According to Theorem 1 by Fang et al. (2023), our EdgePrompt has a comparable universal capability with GPF. Since EdgePrompt+ provides finer edge prompts than EdgePrompt, it will have a stronger universality than EdgePrompt.

5 EXPERIMENTS

5.1 EXPERIMENTAL SETUP

Datasets and downstream tasks. We evaluate the effectiveness of our proposed method on node classification over five public graph datasets, including Cora (Yang et al., 2016), CiteSeer (Yang et al., 2016), Pubmed (Yang et al., 2016), ogbn-arxiv (Hu et al., 2020a), and Flickr (Zeng et al., 2020). In addition, we adopt five graph datasets from TUDataset (Morris et al., 2020), including ENZYMES, DD, NCI1, NCI109, and Mutagenicity, to conduct experiments for graph classification. Basic information and statistics about these datasets can be found in Appendix C.1.

Pre-training strategies. To evaluate the compatibility of our proposed method with various pre-training strategies, we consider four pre-training strategies in our experiments. For contrastive methods, we use GraphCL (You et al., 2020) and SimGRACE (Xia et al., 2022). For generative methods, we use two edge prediction-based methods, i.e., EP-GPPT and EP-GraphPrompt, adopted by GPPT (Sun et al., 2022a) and GraphPrompt (Liu et al., 2023), respectively. We provide detailed descriptions of these pre-training strategies in Appendix C.2.

Baselines. We evaluate our proposed method against five state-of-the-art graph prompt tuning methods in our experiments, including GPPT (Sun et al., 2022a), GraphPrompt (Liu et al., 2023) All-in-one (Sun et al., 2023a), GPF (Fang et al., 2023), and GPF-plus (Fang et al., 2023). Since GPPT is specifically designed for node classification, we only report its performance for node classification tasks. In addition, we also report the performance of solely training classifiers without any prompts (named as *Classifier Only*) in our experiments.

Implementation details. In our experiments, We use a 2-layer GCN (Kipf & Welling, 2017) as the backbone for node classification tasks and a 5-layer GIN (Xu et al., 2019) as the backbone for graph classification tasks. The size of hidden layers is set as 128. The classifier adopted for downstream

Table 2: Accuracy on 5-shot node classification tasks over five datasets. The best-performing method is **bolded** and the runner-up is underlined.

Pre-training Strategies	Tuning Methods	Cora	CiteSeer	Pubmed	ogbn-arxiv	Flickr
GraphCL	Classifier Only	53.05 \pm 4.76	38.62 \pm 3.43	64.28 \pm 4.51	21.15 \pm 1.64	24.32 \pm 2.93
	GPPT	50.96 \pm 6.67	39.50 \pm 1.67	60.47 \pm 4.75	17.99 \pm 1.14	24.35 \pm 1.84
	GraphPrompt	55.71 \pm 4.62	40.81 \pm 2.11	63.47 \pm 2.23	21.03 \pm 1.92	26.08\pm3.44
	ALL-in-one	38.00 \pm 4.17	40.27 \pm 2.09	58.61 \pm 3.49	16.42 \pm 2.98	25.08 \pm 3.44
	GPF	58.52 \pm 4.07	43.55 \pm 2.80	67.67 \pm 3.14	21.73 \pm 1.75	23.98 \pm 1.71
	GPF-plus	52.24 \pm 4.59	38.47 \pm 3.27	64.30 \pm 4.58	21.03 \pm 1.96	25.32 \pm 2.02
	EdgePrompt	58.60 \pm 4.46	43.31 \pm 3.23	67.76\pm3.01	21.90 \pm 1.71	24.83 \pm 2.78
	EdgePrompt+	62.88\pm6.43	46.20\pm0.99	67.41 \pm 5.25	23.18\pm1.26	25.57 \pm 3.04
SimGRACE	Classifier Only	52.27 \pm 2.74	40.45 \pm 3.55	56.72 \pm 3.80	20.75 \pm 2.92	25.53 \pm 3.98
	GPPT	52.07 \pm 7.65	40.25 \pm 3.29	58.65 \pm 5.12	17.76 \pm 1.80	23.37 \pm 4.66
	GraphPrompt	51.42 \pm 2.80	41.74 \pm 2.22	55.98 \pm 2.94	20.48 \pm 2.57	25.88 \pm 3.81
	ALL-in-one	34.64 \pm 4.06	38.95 \pm 2.35	54.18 \pm 4.70	16.72 \pm 2.90	27.68 \pm 4.58
	GPF	58.23 \pm 4.19	44.87 \pm 4.35	61.55 \pm 3.79	21.86 \pm 2.91	26.51 \pm 4.69
	GPF-plus	52.27 \pm 3.34	41.02 \pm 3.49	56.95 \pm 3.86	21.44 \pm 3.77	28.35 \pm 5.50
	EdgePrompt	58.37 \pm 4.51	43.94 \pm 4.15	61.10 \pm 3.69	21.85 \pm 2.54	30.12\pm5.04
	EdgePrompt+	62.40\pm7.97	46.62\pm2.53	64.91\pm5.58	22.74\pm2.34	28.50 \pm 4.08
EP-GPPT	Classifier Only	28.65 \pm 4.82	26.77 \pm 2.03	40.14 \pm 5.69	11.57 \pm 1.91	28.39 \pm 7.44
	GPPT	41.28 \pm 6.92	35.32 \pm 1.27	53.41 \pm 3.99	13.73 \pm 1.16	29.83 \pm 3.73
	GraphPrompt	31.65 \pm 3.33	26.98 \pm 1.24	44.18 \pm 5.57	11.31 \pm 1.89	26.02 \pm 1.16
	ALL-in-one	31.57 \pm 2.16	28.87 \pm 2.57	46.02 \pm 4.23	15.94 \pm 0.75	31.89 \pm 1.14
	GPF	37.56 \pm 3.81	29.74 \pm 1.73	48.86 \pm 7.32	16.95 \pm 1.58	29.68 \pm 6.73
	GPF-plus	28.87 \pm 3.18	26.65 \pm 1.91	40.32 \pm 5.77	11.78 \pm 1.55	29.41 \pm 6.79
	EdgePrompt	37.26 \pm 4.53	29.83 \pm 1.01	47.20 \pm 7.06	17.22 \pm 1.31	31.17 \pm 6.58
	EdgePrompt+	56.41\pm3.62	43.49\pm2.62	61.51\pm4.91	17.78\pm2.16	32.70\pm6.21
EP-GraphPrompt	Classifier Only	59.00 \pm 5.74	44.54 \pm 4.44	72.09 \pm 5.70	31.28 \pm 1.50	27.83 \pm 4.77
	GPPT	54.29 \pm 7.90	45.81 \pm 3.54	66.56 \pm 4.06	25.34 \pm 1.85	28.41 \pm 3.68
	GraphPrompt	60.22 \pm 4.04	47.07 \pm 3.09	73.13 \pm 5.07	32.40 \pm 1.30	28.10 \pm 3.27
	ALL-in-one	42.55 \pm 2.99	44.36 \pm 2.52	67.66 \pm 6.38	15.22 \pm 3.04	31.79 \pm 6.19
	GPF	62.62 \pm 6.40	49.02 \pm 4.53	73.62 \pm 6.42	31.88 \pm 1.08	28.98 \pm 5.30
	GPF-plus	58.23 \pm 5.68	44.60 \pm 4.47	72.15 \pm 5.64	31.58 \pm 1.09	28.96 \pm 4.63
	EdgePrompt	62.74 \pm 6.77	48.69 \pm 4.36	73.60 \pm 5.14	32.67\pm1.83	29.81 \pm 3.59
	EdgePrompt+	64.47\pm7.04	49.71\pm2.25	73.72\pm5.10	31.41 \pm 1.88	32.09\pm4.93

tasks is linear probes for all the methods. We use an Adam optimizer (Kingma & Ba, 2015) with learning rates 0.001 for all the methods. The batch size is set as 32. The number of epochs is set to 200 for graph prompt tuning. The default number of anchor prompts at each GNN layer is 10 for node classification tasks and 5 for graph classification tasks. We use the 5-shot setting for node classification tasks and the 50-shot setting for graph classification tasks. We conduct experiments five times with different random seeds and report the average results in our experiments.

5.2 MAIN RESULTS

We first compare the overall performance of our proposed methods and other baselines. Table 2 reports the results of our method and six baselines on 5-shot node classification tasks over five datasets under four pre-training strategies. According to the table, we observe that our method can consistently achieve the best or most competitive performance among graph prompt tuning methods across different pre-training strategies. Generally, EdgePrompt+ has better performance than EdgePrompt, which is consistent with our analyses in Section 4.3 and validates the necessity of our design on customized edge prompts.

In addition, we conduct experiments on 50-shot graph classification tasks over five datasets under four pre-training strategies and report the results in Table 3. According to the table, we observe that EdgePrompt+ can always get the best place or runner-up for every experimental setting, espe-

Table 3: Accuracy on 50-shot graph classification tasks over five datasets. The best-performing method is **bolded** and the runner-up underlined.

Pre-training Strategies	Tuning Methods	ENZYMES	DD	NCI1	NCI109	Mutagenicity
GraphCL	Classifier Only	30.50 \pm 1.16	62.89 \pm 2.19	62.49 \pm 1.95	61.68 \pm 0.93	66.62 \pm 1.87
	GraphPrompt	27.83 \pm 1.61	64.33 \pm 1.79	63.19 \pm 1.71	62.18 \pm 0.48	67.62\pm0.65
	ALL-in-one	25.92 \pm 0.55	66.54 \pm 1.82	57.52 \pm 2.61	62.74 \pm 0.78	63.43 \pm 2.53
	GPF	30.08 \pm 1.25	64.54 \pm 2.22	62.66 \pm 1.83	62.29 \pm 0.90	66.54 \pm 1.85
	GPF-plus	31.00 \pm 1.50	67.26 \pm 2.29	64.56 \pm 1.10	62.84 \pm 0.22	66.82 \pm 1.63
	EdgePrompt	29.50 \pm 1.57	64.16 \pm 2.13	63.05 \pm 2.11	62.59 \pm 0.93	66.87 \pm 1.88
	EdgePrompt+	34.00\pm1.25	67.98\pm2.05	66.30\pm2.54	66.52\pm0.91	<u>67.47\pm2.37</u>
SimGRACE	Classifier Only	27.07 \pm 1.04	61.77 \pm 2.40	61.27 \pm 3.64	62.12 \pm 1.10	67.36 \pm 0.71
	GraphPrompt	26.87 \pm 1.47	62.58 \pm 1.84	62.45 \pm 1.52	62.41 \pm 0.69	68.03 \pm 0.78
	ALL-in-one	25.73 \pm 1.18	65.16 \pm 1.47	58.52 \pm 1.59	62.01 \pm 0.66	64.43 \pm 1.00
	GPF	28.53 \pm 1.76	65.64 \pm 0.70	61.45 \pm 3.13	61.90 \pm 1.26	67.19 \pm 0.74
	GPF-plus	27.33 \pm 2.01	67.20 \pm 1.56	61.61 \pm 2.89	62.84 \pm 0.23	67.69 \pm 0.64
	EdgePrompt	29.33 \pm 2.30	63.97 \pm 2.14	62.02 \pm 3.02	62.02 \pm 1.03	67.55 \pm 0.85
	EdgePrompt+	32.67\pm2.53	67.72\pm1.62	67.07\pm1.96	66.53\pm1.30	68.31\pm1.36
EP-GPPT	Classifier Only	29.08 \pm 1.35	62.12 \pm 2.82	56.85 \pm 4.35	62.27 \pm 0.78	66.30 \pm 1.78
	GraphPrompt	26.67 \pm 1.60	61.61 \pm 1.91	58.77 \pm 0.97	62.16 \pm 0.89	66.37 \pm 1.17
	ALL-in-one	24.92 \pm 1.33	63.61 \pm 2.12	59.14 \pm 2.12	59.70 \pm 1.37	64.86 \pm 1.60
	GPF	28.33 \pm 1.73	63.48 \pm 2.08	58.14 \pm 4.16	62.52 \pm 1.39	66.10 \pm 0.96
	GPF-plus	29.25 \pm 1.30	66.92\pm2.34	<u>62.93\pm3.23</u>	<u>64.13\pm1.42</u>	<u>67.57\pm1.45</u>
	EdgePrompt	28.33 \pm 3.41	64.03 \pm 2.26	59.85 \pm 3.15	62.98 \pm 1.44	66.36 \pm 1.22
	EdgePrompt+	32.75\pm2.26	66.16 \pm 1.60	63.58\pm2.07	65.15\pm1.60	68.35\pm1.57
EP-GraphPrompt	Classifier Only	31.33 \pm 3.22	62.58 \pm 2.40	62.09 \pm 2.31	60.19 \pm 1.71	65.13 \pm 0.81
	GraphPrompt	30.20 \pm 1.93	64.72 \pm 1.98	62.57 \pm 1.45	62.32 \pm 0.95	<u>65.85\pm0.65</u>
	ALL-in-one	29.07 \pm 1.16	65.60 \pm 2.38	58.67 \pm 2.42	57.69 \pm 1.08	64.66 \pm 0.76
	GPF	30.93 \pm 1.76	66.21 \pm 1.66	61.80 \pm 2.78	62.27 \pm 1.18	65.61 \pm 0.59
	GPF-plus	30.67 \pm 3.06	67.50\pm2.45	<u>62.59\pm2.09</u>	61.98 \pm 1.60	65.51 \pm 1.10
	EdgePrompt	30.80 \pm 2.09	65.87 \pm 1.35	61.75 \pm 2.49	62.33 \pm 1.65	65.77 \pm 0.90
	EdgePrompt+	33.27\pm2.71	<u>67.47\pm2.14</u>	65.06\pm1.84	64.64\pm1.57	66.42\pm1.31

cially over ENZYMES, NCI1, and NCI109. In addition, we observe that GPF and EdgePrompt have relatively small performance gaps (always $< 1.8\%$) in the table (we also observe this in node classification tasks). As indicated in Theorem 2, our proposed EdgePrompt has a comparable universal capability with GPF to achieve graph representations equivalent to any graph transformation. These observations effectively support our theoretical claim in this study.

5.3 CONVERGENCE ANALYSIS

In this subsection, we would like to investigate the convergence speeds of our method compared with baselines. Figure 2 illustrates the accuracy curves of our method and the baselines under two pre-training strategies. According to Figure 2, we can observe that EdgePrompt+ can generally converge faster than other methods.

5.4 INFLUENCE OF PROMPT NUMBERS

We conduct experiments to investigate the impact of different numbers of anchor prompts on model utility. Figure 3 and Figure 4 illustrate the performance of EdgePrompt+ with 1, 5, 10, 20, and 50 anchor prompts at each layer for node classification and graph classification tasks, respectively. Note that EdgePrompt+ will be degraded to EdgePrompt when we have only one anchor prompt at each GNN layer. From the two figures, we can conclude only one anchor prompt vector (i.e., EdgePrompt) is insufficient in most cases where each edge will learn a global prompt vector. In the meantime, EdgePrompt+ with too many anchor prompts (e.g., 50) may not further improve the performance. We recommend 5 or 10 as the initial number of anchor prompts.

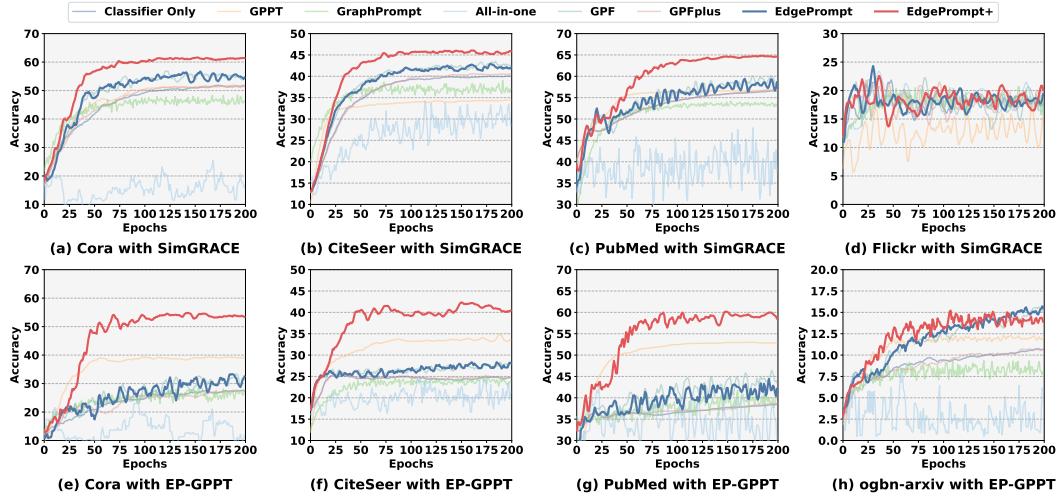


Figure 2: Convergence speeds of different methods.

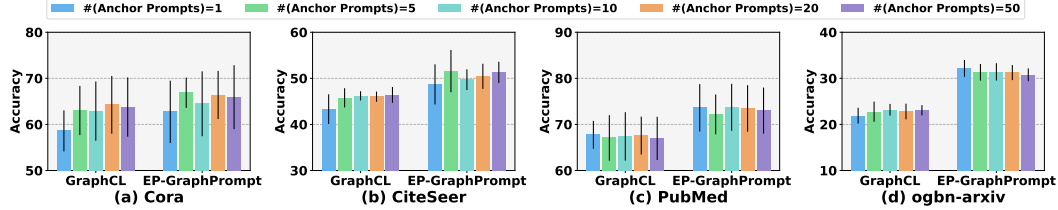


Figure 3: Results of EdgePrompt+ with varying numbers of anchor prompts on node classification.

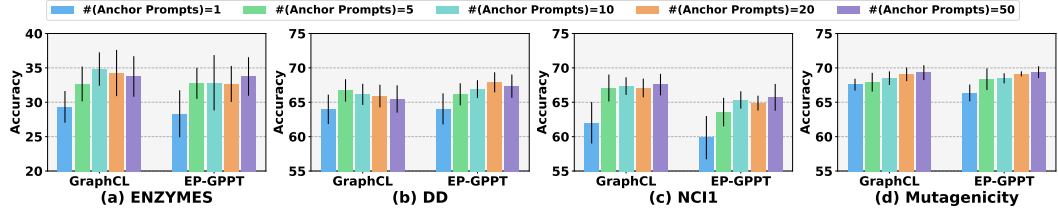


Figure 4: Results of EdgePrompt+ with varying numbers of anchor prompts on graph classification.

6 CONCLUSION

Graph prompt tuning is an emerging technique to bridge the objective gap between pre-training and downstream tasks. Unlike previous studies focusing on designing prompts on nodes, we propose a simple yet effective method, EdgePrompt and its variant EdgePrompt+, that manipulates the input graph by adding extra learnable prompt vectors to edges and thereby obtaining a prompted graph suitable for downstream tasks. We provide comprehensive theoretical analyses of our method regarding its capability of handling node classification and graph classification. We conduct extensive experiments over ten graph datasets under four pre-training strategies. Experiment results demonstrate the superiority of our method compared with six baselines.

REPRODUCIBILITY STATEMENT

The datasets adopted in our experiments are public graph datasets and can be downloaded from the Web. Our code is available at the anonymous link: <https://anonymous.4open.science/r/EdgePrompt-4905>. We provide implementation details in Section 5.1 to help readers reproduce the results.

REFERENCES

- Hyojin Bahng, Ali Jahanian, Swami Sankaranarayanan, and Phillip Isola. Exploring visual prompts for adapting large-scale models. *arXiv preprint arXiv:2203.17274*, 2022.
- Shaked Brody, Uri Alon, and Eran Yahav. How attentive are graph attention networks? In *International Conference on Learning Representations*, 2022.
- Ming Chen, Zhewei Wei, Zengfeng Huang, Bolin Ding, and Yaliang Li. Simple and deep graph convolutional networks. In *International conference on machine learning*, 2020.
- Limeng Cui, Haeseung Seo, Maryam Tabar, Fenglong Ma, Suhan Wang, and Dongwon Lee. De-terrent: Knowledge guided graph attention network for detecting healthcare misinformation. In *Proceedings of the 26th ACM SIGKDD international conference on knowledge discovery & data mining*, 2020.
- Taoran Fang, Yunchao Zhang, Yang Yang, Chunping Wang, and Lei Chen. Universal prompt tuning for graph neural networks. *Advances in Neural Information Processing Systems*, 2023.
- Bahare Fatemi, Layla El Asri, and Seyed Mehran Kazemi. Slaps: Self-supervision improves structure learning for graph neural networks. *Advances in Neural Information Processing Systems*, 2021.
- Johannes Gasteiger, Stefan Weißenberger, and Stephan Günnemann. Diffusion improves graph learning. *Advances in neural information processing systems*, 2019.
- Liyu Gong and Qiang Cheng. Exploiting edge features for graph neural networks. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, 2019.
- Will Hamilton, Zhitaoying, and Jure Leskovec. Inductive representation learning on large graphs. In *Advances in neural information processing systems*, 2017.
- Zhenyu Hou, Xiao Liu, Yukuo Cen, Yuxiao Dong, Hongxia Yang, Chunjie Wang, and Jie Tang. Graphmae: Self-supervised masked graph autoencoders. In *Proceedings of the 28th ACM SIGKDD Conference on Knowledge Discovery and Data Mining*, 2022.
- Weihua Hu, Matthias Fey, Marinka Zitnik, Yuxiao Dong, Hongyu Ren, Bowen Liu, Michele Catasta, and Jure Leskovec. Open graph benchmark: Datasets for machine learning on graphs. *Advances in neural information processing systems*, 2020a.
- Weihua Hu, Bowen Liu, Joseph Gomes, Marinka Zitnik, Percy Liang, Vijay Pande, and Jure Leskovec. Strategies for pre-training graph neural networks. In *International Conference on Learning Representations*, 2020b.
- Ziniu Hu, Changjun Fan, Ting Chen, Kai-Wei Chang, and Yizhou Sun. Pre-training graph neural networks for generic structural feature extraction. *arXiv preprint arXiv:1905.13728*, 2019.
- Renhong Huang, Jiarong Xu, Xin Jiang, Chenglu Pan, Zhiming Yang, Chunping Wang, and Yang Yang. Measuring task similarity and its implication in fine-tuning graph neural networks. In *Proceedings of the AAAI Conference on Artificial Intelligence*, 2024.
- Xiaodong Jiang, Ronghang Zhu, Sheng Li, and Pengsheng Ji. Co-embedding of nodes and edges with graph neural networks. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 2020.
- Wei Jin, Tyler Derr, Haochen Liu, Yiqi Wang, Suhan Wang, Zitao Liu, and Jiliang Tang. Self-supervised learning on graphs: Deep insights and new direction. *arXiv preprint arXiv:2006.10141*, 2020.
- Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. In *International Conference on Learning Representations*, 2015.
- Thomas N Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. In *International Conference on Learning Representations*, 2017.

- Xin Liu, Jiayang Cheng, Yangqiu Song, and Xin Jiang. Boosting graph structure learning with dummy nodes. In *International Conference on Machine Learning*, 2022a.
- Yanbei Liu, Henan Li, Tao Luo, Changqing Zhang, Zhitao Xiao, Ying Wei, Yaozong Gao, Feng Shi, Fei Shan, and Dinggang Shen. Structural attention graph neural network for diagnosis and prediction of covid-19 severity. *IEEE Transactions on Medical Imaging*, 2022b.
- Yixin Liu, Yu Zheng, Daokun Zhang, Hongxu Chen, Hao Peng, and Shirui Pan. Towards unsupervised deep graph structure learning. In *Proceedings of the ACM Web Conference 2022*, 2022c.
- Zemin Liu, Xingtong Yu, Yuan Fang, and Xinming Zhang. Graphprompt: Unifying pre-training and downstream tasks for graph neural networks. In *Proceedings of the ACM Web Conference 2023*, 2023.
- Yao Ma, Xiaorui Liu, Neil Shah, and Jiliang Tang. Is homophily a necessity for graph neural networks? In *International Conference on Learning Representations*, 2022.
- Yihong Ma, Ning Yan, Jiayu Li, Masood Mortazavi, and Nitesh V Chawla. Hetgpt: Harnessing the power of prompt tuning in pre-trained heterogeneous graph neural networks. In *Proceedings of the ACM on Web Conference 2024*, 2024.
- Christopher Morris, Nils M Kriege, Franka Bause, Kristian Kersting, Petra Mutzel, and Marion Neumann. TUDataset: A collection of benchmark datasets for learning with graphs. *arXiv preprint arXiv:2007.08663*, 2020.
- Emanuele Rossi, Ben Chamberlain, Fabrizio Frasca, Davide Eynard, Federico Monti, and Michael Bronstein. Temporal graph networks for deep learning on dynamic graphs. *arXiv preprint arXiv:2006.10637*, 2020.
- Michael Schlichtkrull, Thomas N Kipf, Peter Bloem, Rianne van den Berg, Ivan Titov, and Max Welling. Modeling relational data with graph convolutional networks. In *15th International Conference on Extended Semantic Web Conference*, 2018.
- Weijing Shi and Raj Rajkumar. Point-gnn: Graph neural network for 3d object detection in a point cloud. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, 2020.
- Fan-Yun Sun, Jordan Hoffmann, Vikas Verma, and Jian Tang. Infograph: Unsupervised and semi-supervised graph-level representation learning via mutual information maximization. In *International Conference on Learning Representations*, 2020.
- Mingchen Sun, Kaixiong Zhou, Xin He, Ying Wang, and Xin Wang. Gppt: Graph pre-training and prompt tuning to generalize graph neural networks. In *Proceedings of the 28th ACM SIGKDD Conference on Knowledge Discovery and Data Mining*, 2022a.
- Qingyun Sun, Jianxin Li, Hao Peng, Jia Wu, Xingcheng Fu, Cheng Ji, and S Yu Philip. Graph structure learning with variational information bottleneck. In *Proceedings of the AAAI Conference on Artificial Intelligence*, 2022b.
- Xiangguo Sun, Hong Cheng, Jia Li, Bo Liu, and Jihong Guan. All in one: Multi-task prompting for graph neural networks. In *Proceedings of the 29th ACM SIGKDD Conference on Knowledge Discovery and Data Mining*, 2023a.
- Xiangguo Sun, Jiawen Zhang, Xixi Wu, Hong Cheng, Yun Xiong, and Jia Li. Graph prompt learning: A comprehensive survey and beyond. *arXiv preprint arXiv:2311.16534*, 2023b.
- Yifei Sun, Qi Zhu, Yang Yang, Chunping Wang, Tianyu Fan, Jiajun Zhu, and Lei Chen. Fine-tuning graph neural networks by preserving graph generative patterns. In *Proceedings of the AAAI Conference on Artificial Intelligence*, 2024.
- Zhen Tan, Ruocheng Guo, Kaize Ding, and Huan Liu. Virtual node tuning for few-shot node classification. In *Proceedings of the 29th ACM SIGKDD Conference on Knowledge Discovery and Data Mining*, 2023.

- Anton Tsitsulin, Benedek Rozemberczki, John Palowitch, and Bryan Perozzi. Synthetic graph generation to benchmark graph learning. *arXiv preprint arXiv:2204.01376*, 2022.
- Shikhar Vashishth, Soumya Sanyal, Vikram Nitin, and Partha Talukdar. Composition-based multi-relational graph convolutional networks. In *International Conference on Learning Representations*, 2020.
- Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, and Yoshua Bengio. Graph attention networks. In *International Conference on Learning Representations*, 2018.
- Petar Veličković, William Fedus, William L Hamilton, Pietro Liò, Yoshua Bengio, and R Devon Hjelm. Deep graph infomax. In *International Conference on Learning Representations*, 2019.
- Yue Wang, Yongbin Sun, Ziwei Liu, Sanjay E Sarma, Michael M Bronstein, and Justin M Solomon. Dynamic graph cnn for learning on point clouds. *ACM Transactions on Graphics (tog)*, 2019.
- Xuemei Wei, Yezheng Liu, Jianshan Sun, Yuanchun Jiang, Qifeng Tang, and Kun Yuan. Dual subgraph-based graph neural network for friendship prediction in location-based social networks. *ACM Transactions on Knowledge Discovery from Data*, 2023.
- Felix Wu, Amauri Souza, Tianyi Zhang, Christopher Fifty, Tao Yu, and Kilian Weinberger. Simplifying graph convolutional networks. In *International conference on machine learning*, 2019.
- Junyang Wu, Xianhang Li, Chen Wei, Huiyu Wang, Alan Yuille, Yuyin Zhou, and Cihang Xie. Unleashing the power of visual prompting at the pixel level. *arXiv preprint arXiv:2212.10556*, 2022.
- Zhenqin Wu, Bharath Ramsundar, Evan N Feinberg, Joseph Gomes, Caleb Geniesse, Aneesh S Pappu, Karl Leswing, and Vijay Pande. Moleculenet: a benchmark for molecular machine learning. *Chemical science*, 2018.
- Jun Xia, Lirong Wu, Jintao Chen, Bozhen Hu, and Stan Z Li. Simgrace: A simple framework for graph contrastive learning without data augmentation. In *Proceedings of the ACM Web Conference 2022*, 2022.
- Jiarong Xu, Renhong Huang, Xin Jiang, Yuxuan Cao, Carl Yang, Chunping Wang, and Yang Yang. Better with less: A data-active perspective on pre-training graph neural networks. *Advances in Neural Information Processing Systems*, 2023.
- Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. How powerful are graph neural networks? In *International Conference on Learning Representations*, 2019.
- Liang Yang, Mengzhe Li, Liyang Liu, Chuan Wang, Xiaochun Cao, Yuanfang Guo, et al. Diverse message passing for attribute with heterophily. *Advances in Neural Information Processing Systems*, 2021.
- Yulei Yang and Dongsheng Li. Nenn: Incorporate node and edge features in graph neural networks. In *Asian conference on machine learning*, 2020.
- Zhilin Yang, William Cohen, and Ruslan Salakhudinov. Revisiting semi-supervised learning with graph embeddings. In *International conference on machine learning*, 2016.
- Yuning You, Tianlong Chen, Yongduo Sui, Ting Chen, Zhangyang Wang, and Yang Shen. Graph contrastive learning with augmentations. *Advances in neural information processing systems*, 2020.
- Xingtong Yu, Yuan Fang, Zemin Liu, and Xinming Zhang. Hgprompt: Bridging homogeneous and heterogeneous graphs for few-shot prompt learning. In *Proceedings of the AAAI Conference on Artificial Intelligence*, 2024a.
- Xingtong Yu, Zhenghao Liu, Yuan Fang, Zemin Liu, Sihong Chen, and Xinming Zhang. Generalized graph prompt: Toward a unification of pre-training and downstream tasks on graphs. *IEEE Transactions on Knowledge and Data Engineering*, 2024b.

- Xingtong Yu, Jie Zhang, Yuan Fang, and Renhe Jiang. Non-homophilic graph pre-training and prompt learning. *arXiv preprint arXiv:2408.12594*, 2024c.
- Xingtong Yu, Chang Zhou, Yuan Fang, and Xinming Zhang. Multigprompt for multi-task pre-training and prompting on graphs. In *Proceedings of the ACM on Web Conference 2024*, 2024d.
- Hanqing Zeng, Hongkuan Zhou, Ajitesh Srivastava, Rajgopal Kannan, and Viktor Prasanna. Graph-saint: Graph sampling based inductive learning method. In *International Conference on Learning Representations*, 2020.
- Yifei Zhang, Hao Zhu, Zixing Song, Piotr Koniusz, and Irwin King. Spectral feature augmentation for graph contrastive learning and beyond. In *Proceedings of the AAAI Conference on Artificial Intelligence*, 2023.
- WANG Zhili, DI Shimin, CHEN Lei, and ZHOU Xiaofang. Search to fine-tune pre-trained graph neural networks for graph-level tasks. In *2024 IEEE 40th International Conference on Data Engineering (ICDE)*, 2024.
- Haoran Zhou, Yidan Feng, Mingsheng Fang, Mingqiang Wei, Jing Qin, and Tong Lu. Adaptive graph convolution for point cloud analysis. In *Proceedings of the IEEE/CVF international conference on computer vision*, 2021.
- Kaiyang Zhou, Jingkang Yang, Chen Change Loy, and Ziwei Liu. Conditional prompt learning for vision-language models. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, 2022.
- Zhilun Zhou, Yu Liu, Jingtao Ding, Depeng Jin, and Yong Li. Hierarchical knowledge graph learning enabled socioeconomic indicator prediction in location-based social network. In *Proceedings of the ACM Web Conference*, 2023.
- Chenyi Zi, Haihong Zhao, Xiangguo Sun, Yiqing Lin, Hong Cheng, and Jia Li. Prog: A graph prompt learning benchmark. *arXiv preprint arXiv:2406.05346*, 2024.

A PROOF OF THEOREM 1

Theorem 1. Given a random graph $\mathcal{G} \sim CSBM(\mu_1, \mu_2, p, q)$ and a pre-trained GCN model f , there always exist a set of $M \geq 2$ anchor prompts $\mathcal{P} = \{\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_M\}$ and the score vectors $\mathbf{b}_{i,j}$ for each edge (v_i, v_j) that improve the expected distance after GCN operation between classes c_1 and c_2 to T times without using edge prompts, where $T \in (1, 1 + \frac{p}{|p-q|}]$.

Proof. For each node v_i in graph \mathcal{G} , we can approximately regard that the labels of its neighboring nodes are independently sampled from a neighborhood distribution $\mathcal{D}_{c_1} = [\frac{p}{p+q}, \frac{q}{p+q}]$ if node v_i is in class c_1 or $\mathcal{D}_{c_2} = [\frac{q}{p+q}, \frac{p}{p+q}]$ if node v_i is in class c_2 (Ma et al., 2022). When we do not consider edge prompts, the expected feature obtained from the GCN operation will be

$$\mathbb{E}[\mathbf{h}_1] = \frac{p}{p+q} \cdot \mu_1 + \frac{q}{p+q} \cdot \mu_2 \quad (10)$$

for nodes in class c_1 and

$$\mathbb{E}[\mathbf{h}_2] = \frac{q}{p+q} \cdot \mu_1 + \frac{p}{p+q} \cdot \mu_2 \quad (11)$$

for nodes in class c_2 . Here, we ignore the linear transformation in the GCN operation since it can be absorbed by the linear classifier. To evaluate the linear separability of linear classifiers, we calculate the expected distance d between the two classes c_1 and c_2 by

$$d = \|\mathbb{E}[\mathbf{h}_1] - \mathbb{E}[\mathbf{h}_2]\| = \frac{|p-q|}{p+q} \cdot \|\mu_1 - \mu_2\|. \quad (12)$$

When we consider edge prompts in EdgePrompt+, we need to involve them into the aggregation in the GCN operation. Without loss of generality, we can fix $b_{ijm} = 0$ for $m \in [3, M]$. Therefore, for each edge (v_i, v_j) , its prompt vector will be

$$\mathbf{e}_{ij} = \sum_{m=1}^{M_1} b_{ijm} \cdot \mathbf{p}_m = b_{ij1} \cdot \mathbf{p}_1 + b_{ij2} \cdot \mathbf{p}_2. \quad (13)$$

Obviously, $b_{ij2} = 1 - b_{ij1}$. In addition, we can set the two prompt vectors as $\boldsymbol{\mu}_1$ and $\boldsymbol{\mu}_2$, i.e.,

$$\mathbf{e}_{ij} = b_{ij1} \cdot \boldsymbol{\mu}_1 + b_{ij2} \cdot \boldsymbol{\mu}_2. \quad (14)$$

Then the new expected feature obtained from the GCN operation with edge prompts will be

$$\mathbb{E}[\mathbf{h}'_1] = \frac{p \cdot (\boldsymbol{\mu}_1 + b_{11} \cdot \boldsymbol{\mu}_1 + (1 - b_{11}) \cdot \boldsymbol{\mu}_2) + q \cdot (\boldsymbol{\mu}_2 + b_{12} \cdot \boldsymbol{\mu}_1 + (1 - b_{12}) \cdot \boldsymbol{\mu}_2)}{p + q} \quad (15)$$

for nodes in class c_1 and

$$\mathbb{E}[\mathbf{h}'_2] = \frac{q \cdot (\boldsymbol{\mu}_1 + b_{21} \cdot \boldsymbol{\mu}_1 + (1 - b_{21}) \cdot \boldsymbol{\mu}_2) + p \cdot (\boldsymbol{\mu}_2 + b_{22} \cdot \boldsymbol{\mu}_1 + (1 - b_{22}) \cdot \boldsymbol{\mu}_2)}{p + q} \quad (16)$$

for nodes in class c_2 . Here, $b_{11} \in [0, 1]$ represents the expected score between nodes from class 1, $b_{22} \in [0, 1]$ represents the expected score between nodes from class 2, $b_{12} \in [0, 1]$ and $b_{21} \in [0, 1]$ represents the expected score between nodes across classes. Different from the original design in our method, we can set $b_{12} = b_{21}$ for simplicity. Therefore, the new expected distance with edge prompts will be

$$\begin{aligned} d' &= \|\mathbb{E}[\mathbf{h}'_1] - \mathbb{E}[\mathbf{h}'_2]\| \\ &= \left\| \frac{(p - q + b_{11} \cdot p - b_{22} \cdot p)\boldsymbol{\mu}_1 - (-(1 - b_{11}) \cdot p - q + p + (1 - b_{22}) \cdot p)\boldsymbol{\mu}_2}{p + q} \right\| \\ &= \frac{|(p - q + (b_{11} - b_{22}) \cdot p)|}{p + q} \cdot \|\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2\| \end{aligned} \quad (17)$$

To improve the linear separability of the two classes, we hope to get $d' > d$. In this case, we may assume

$$d' = T \cdot d = \frac{|T \cdot (p - q)|}{p + q} \cdot \|\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2\| \quad (18)$$

with $T > 1$. Therefore, we need

$$b_{11} - b_{22} = \frac{(T - 1) \cdot (p - q)}{p}. \quad (19)$$

Since $b_{11} \in [0, 1]$ and $b_{22} \in [0, 1]$, we need

$$-1 \leq \frac{(T - 1) \cdot (p - q)}{p} \leq 1. \quad (20)$$

Then we have

$$T \leq 1 + \frac{p}{|p - q|}. \quad (21)$$

Therefore, We can conclude that we can always find a set of $M \geq 2$ anchor prompts $\mathcal{P} = \{\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \mathbf{p}_3, \dots, \mathbf{p}_M\}$ and the above score values for each edge (v_i, v_j) that improve the expected distance after GCN operation between classes c_1 and c_2 to T times without using edge prompts, where $T \in (1, 1 + \frac{p}{|p - q|}]$. \square

B PROOF OF THEOREM 2

Before we prove Theorem 2, we would like to prove the following lemma.

Lemma 1. *Given an input graph $\mathcal{G} = (\mathbf{X}, \mathbf{A})$ and an extra feature prompt $\hat{\mathbf{p}}$ in GPF, there exists a set of edge prompt vectors $\{\mathbf{p}^{(1)}, \mathbf{p}^{(2)}, \dots, \mathbf{p}^{(L)}\}$ in EdgePrompt that can satisfy*

$$f(\mathbf{X}, \mathbf{A}, \{\mathbf{p}^{(1)}, \dots, \mathbf{p}^{(L)}\}) = f(\mathbf{X} + \hat{\mathbf{p}}, \mathbf{A}) \quad (22)$$

for any pre-trained GNN model f .

Proof. Following GPF (Fang et al., 2023), we first consider a single-layer GIN (Xu et al., 2019) with a linear transformation. Mathematically, we can compute the node representation matrix in a GIN layer by

$$\mathbf{H} = (\mathbf{A} + (1 + \epsilon) \cdot \mathbf{I}) \cdot \mathbf{X} \cdot \mathbf{W} = \mathbf{A} \cdot \mathbf{X} \cdot \mathbf{W} + (1 + \epsilon) \cdot \mathbf{X} \cdot \mathbf{W}. \quad (23)$$

In GPF, the feature prompt $\hat{\mathbf{p}}$ is added to the feature vector for each node. Then the new node representation matrix with $\hat{\mathbf{p}}$ can be written as

$$\begin{aligned} \mathbf{H}_{\hat{\mathbf{p}}} &= (\mathbf{A} + (1 + \epsilon) \cdot \mathbf{I}) \cdot (\mathbf{X} + [\mathbf{1}]^N \cdot \hat{\mathbf{p}}) \cdot \mathbf{W} \\ &= (\mathbf{A} + (1 + \epsilon) \cdot \mathbf{I}) \cdot \mathbf{X} \cdot \mathbf{W} + (\mathbf{A} + (1 + \epsilon) \cdot \mathbf{I}) \cdot [\mathbf{1}]^N \cdot \hat{\mathbf{p}} \cdot \mathbf{W} \\ &= \mathbf{H} + (\mathbf{A} + (1 + \epsilon) \cdot \mathbf{I}) \cdot [\mathbf{1}]^N \cdot \hat{\mathbf{p}} \cdot \mathbf{W} \\ &= \mathbf{H} + [\text{Deg}_i + 1 + \epsilon]^N \cdot \hat{\mathbf{p}} \cdot \mathbf{W} \end{aligned} \quad (24)$$

where $[\mathbf{1}]^N \in \mathbb{R}^{N \times 1}$ represents an N-dimensional column vector with values of 1, $[\text{Deg}_i + 1 + \epsilon]^N \in \mathbb{R}^{N \times 1}$ represents an N-dimensional column vector with the value of i -th row is $\text{Deg}_i + 1 + \epsilon$, and Deg_i represents the degree of node v_i .

In EdgePrompt, the prompt vector will be associated with each edge. Therefore, we can write the node representation matrix with edge prompt \mathbf{p} by

$$\begin{aligned} \mathbf{H}_{\mathbf{p}} &= \mathbf{A} \cdot (\mathbf{X} + [\mathbf{1}]^N \cdot \mathbf{p}) \cdot \mathbf{W} + (1 + \epsilon) \cdot \mathbf{X} \cdot \mathbf{W} \\ &= \mathbf{A} \cdot \mathbf{X} \cdot \mathbf{W} + \mathbf{A} \cdot [\mathbf{1}]^N \cdot \mathbf{p} \cdot \mathbf{W} + (1 + \epsilon) \cdot \mathbf{X} \cdot \mathbf{W} \\ &= \mathbf{H} + \mathbf{A} \cdot [\mathbf{1}]^N \cdot \mathbf{p} \cdot \mathbf{W} \\ &= \mathbf{H} + [\text{Deg}_i]^N \cdot \mathbf{p} \cdot \mathbf{W} \end{aligned} \quad (25)$$

To obtain the same graph representation, we have

$$\text{Sum}(\mathbf{H}_{\hat{\mathbf{p}}}) = \text{Sum}(\mathbf{H}_{\mathbf{p}}), \quad (26)$$

where $\text{Sum}(\mathbf{H})$ computes the sum vector for each row vector of a matrix. We can simplify the above equation by

$$\begin{aligned} \text{Sum}(\mathbf{H}_{\hat{\mathbf{p}}}) &= \text{Sum}(\mathbf{H}_{\mathbf{p}}) \\ &\Rightarrow \text{Sum}(\mathbf{H} + [\text{Deg}_i + 1 + \epsilon]^N \cdot \hat{\mathbf{p}} \cdot \mathbf{W}) = \text{Sum}(\mathbf{H} + [\text{Deg}_i]^N \cdot \mathbf{p} \cdot \mathbf{W}) \\ &\Rightarrow \text{Sum}([\text{Deg}_i + 1 + \epsilon]^N \cdot \hat{\mathbf{p}} \cdot \mathbf{W}) = \text{Sum}([\text{Deg}_i]^N \cdot \mathbf{p} \cdot \mathbf{W}) \\ &\Rightarrow (\text{Deg} + N + N \cdot \epsilon) \cdot \hat{\mathbf{p}} \cdot \mathbf{W} = \text{Deg} \cdot \mathbf{p} \cdot \mathbf{W} \end{aligned} \quad (27)$$

where $\text{Deg} = \sum_{v_i \in \mathcal{G}_V} \text{Deg}_i$. To obtain the above equation, we only need

$$\mathbf{p} = \frac{\text{Deg} + N + N \cdot \epsilon}{\text{Deg}} \cdot \hat{\mathbf{p}}. \quad (28)$$

Therefore, for any feature prompt $\hat{\mathbf{p}}$, we can always find an edge prompt \mathbf{p} in Equation (28) that satisfies Lemma 1.

Extension to other GNN backbones. Various GNN backbones can be expressed as $\mathbf{H} = \mathbf{S} \cdot \mathbf{X} \cdot \mathbf{W}$, where \mathbf{S} is the diffusion matrix (Gasteiger et al., 2019). Different \mathbf{S} only impact the coefficient before $\hat{\mathbf{p}}$ in Equation (28).

Extension to multi-layer GNN models. For multi-layer linear GNN models, the diffusion matrix $\mathbf{S}^{(l)}$ at each layer can be integrated as one overall \mathbf{S} . \square

Theorem 2. Given an input graph $\mathcal{G} = (\mathbf{X}, \mathbf{A})$ and its transformation $\mathcal{G}' = (\mathbf{X}', \mathbf{A}')$ by an arbitrary transformation function \mathcal{T} , there exists a set of edge prompt vectors $\{\mathbf{p}^{(1)}, \mathbf{p}^{(2)}, \dots, \mathbf{p}^{(L)}\}$ in EdgePrompt that can satisfy

$$f(\mathbf{X}, \mathbf{A}, \{\mathbf{p}^{(1)}, \dots, \mathbf{p}^{(L)}\}) = f(\mathbf{X}', \mathbf{A}') \quad (29)$$

for any pre-trained GNN model f .

Table 4: Basic information and statistics of graph datasets adopted in our experiments.

Dataset	#(Graphs)	#(Nodes)	#(Edges)	#(Features)	#(Classes)	Task Level
Cora	1	2,708	10,556	1,433	7	Node
CiteSeer	1	3,327	9,104	3,703	6	Node
Pubmed	1	19,717	88,648	500	3	Node
Flickr	1	89,250	899,756	500	7	Node
ogbn-arxiv	1	169,343	1,166,243	128	40	Node

Dataset	#(Graphs)	#(Avg. Nodes)	#(Avg. Edges)	#(Features)	#(Classes)	Task Level
ENZYMES	600	32.63	124.27	3	6	Graph
DD	1,178	284.32	1,431.32	89	2	Graph
NCI1	4,110	29.87	64.60	37	2	Graph
NCI109	4,127	29.68	64.26	38	2	Graph
Mutagenicity	4,337	30.32	61.54	14	2	Graph

Proof. Given any feature prompts, Lemma 1 indicates that we can always find edge prompts that lead to the same representation of a graph for any pre-trained GNN models. Given Theorem 1 by (Fang et al., 2023), the input graph with a learnable feature prompt can always obtain the same representation as those of any transformed graphs. Therefore, we can conclude that our edge prompts in EdgePrompt have the capacity to obtain the representation equal to those of any transformed graphs for any pre-trained GNN models. \square

C MORE DETAILS ABOUT EXPERIMENTAL SETUP

C.1 DATASETS

Table 4 shows the basic information and statistics of graph datasets adopted in our experiments.

C.2 PRE-TRAINING STRATEGIES

We provide more details about the four pre-training strategies adopted in our experiments.

- **GraphCL** (You et al., 2020) is a contrastive method for pre-training GNN models. The intuition of GraphCL is to maximize the agreement between two views of a graph perturbed by different data augmentations. We adopt node dropping and edge perturbation to generate two graph views. A GNN model generates two graph representations of the same graph. A nonlinear projection head will map the two graph representations to another latent space. The contrastive loss will be used to optimize the GNN model and the projection head.
- **SimGRACE** (Xia et al., 2022) is an augmentation-free contrastive method for GNN pre-training. We first construct a perturbed version of the GNN model by adding noise sampled from the Gaussian distribution. Given an input graph, the perturbed GNN model will generate its representation that forms a positive pair with that generated by the original GNN model.
- **EP-GPPT** (Sun et al., 2022a) pre-trains a GNN model using edge prediction. A set of edges in the original graph is randomly masked. The pre-training task is to predict whether a node pair is connected. Unconnected node pairs are randomly selected to form the negative samples in pre-training.
- **EP-GraphPrompt** (Liu et al., 2023) similarly uses edge prediction for GNN pre-training. Given a node in the input graph, we randomly sample one positive node from its neighbors and one negative node that does not link to it. The pre-training task is to maximize the similarity between the connected nodes while minimizing the similarity between the unconnected nodes.

Table 5: Average running time (seconds per epoch) on 5-shot node classification tasks over five datasets.

Tuning Methods	Cora	CiteSeer	Pubmed	ogbn-arxiv	Flickr
Classifier Only	0.116	0.136	0.663	1.186	5.156
GPPT	0.141	0.151	0.713	1.381	5.828
GraphPrompt	0.126	0.136	0.673	1.377	4.362
All-in-one	0.477	0.578	3.090	6.085	7.357
GPF	0.121	0.131	0.678	1.070	3.482
GPF-plus	0.116	0.131	0.668	1.075	3.427
EdgePrompt	0.121	0.136	0.693	1.106	3.824
EdgePrompt+	0.146	0.156	0.804	1.377	5.894

Table 6: Average running time (seconds per epoch) on 50-shot graph classification tasks over five datasets.

Tuning Methods	ENZYMES	DD	NCI1	NCI109	Mutagenicity
Classifier Only	0.216	0.176	0.291	0.332	0.302
GraphPrompt	0.276	0.211	0.347	0.357	0.322
All-in-one	0.457	0.643	1.337	1.397	1.206
GPF	0.221	0.191	0.342	0.322	0.307
GPF-plus	0.231	0.191	0.347	0.296	0.312
EdgePrompt	0.226	0.196	0.347	0.296	0.317
EdgePrompt+	0.332	0.302	0.442	0.382	0.402

D MORE EXPERIMENTAL RESULTS

D.1 RESULTS ON MODEL EFFICIENCY

Table 5 and Table 6 provide the average running time (seconds per epoch) for node classification and graph classification, respectively. From the two tables, we can observe that most graph prompt tuning method has similar computing time except All-in-one. All-in-one needs more time per epoch since it uses alternating strategies. EdgePrompt has almost the same efficiency as Classifier only without any prompts. In addition, EdgePrompt+ does not introduce significant computational cost.

D.2 RESULTS ON GRAPH DATA WITH EDGE FEATURES

In our experiments, we conduct experiments over graph data without edge features. However, in the real world, many graphs may inherently have edge features. Our method is still compatible with this case. We report the performance of our method and other baselines over BACE and BBBP from the MoleculeNet dataset (Wu et al., 2018) in Table 7. From the table, we can observe that our method can outperform other baselines over the two datasets under two pre-training strategies.

D.3 RESULTS WITH EDGE PROMPTS AT THE FIRST LAYER

Unlike previous studies, we learn prompt vectors at each layer of the pre-trained GNN model. This strategy can consistently avoid adverse information aggregated from different classes. For example, node v_3 in Figure 1 may receive adverse information from node v_1 when node v_3 and node v_1 are from different classes. If we learn edge prompts only at the first layer, node v_3 will still receive adverse information from node v_1 at the following layers. In contrast, our method in EdgePrompt+ instead learns layer-wise edge prompts, which can consistently avoid the above issue at each layer. We conduct experiments on our methods with edge prompts only at the first layer. Table 8 and Table 9 show the performance for node classification and graph classification, respectively. From the tables, we observe performance degradation in most cases, especially for EdgePrompt+. This observation validates our design of learning edge prompts at each layer of the pre-trained GNN model.

Table 7: Accuracy on 50-shot graph classification tasks over two datasets with edge features. The best-performing method is **bolded** and the runner-up underlined.

Pre-training Strategies	Tuning Methods	BACE	BBBP
SimGRACE	Classifier Only	57.62 \pm 1.92	63.56 \pm 1.03
	GraphPrompt	59.37 \pm 0.53	63.39 \pm 1.75
	All-in-one	<u>56.73\pm1.33</u>	<u>65.72\pm3.48</u>
	GPF	57.36 \pm 1.52	<u>63.89\pm1.66</u>
	GPF-plus	57.16 \pm 2.21	64.17 \pm 1.29
	EdgePrompt	58.12 \pm 1.04	63.89 \pm 1.26
	EdgePrompt+	60.46\pm2.63	70.50\pm1.92
EP-GraphPrompt	Classifier Only	60.40 \pm 1.03	66.17 \pm 1.15
	GraphPrompt	<u>61.69\pm1.36</u>	66.86 \pm 0.70
	All-in-one	<u>56.17\pm1.54</u>	61.72 \pm 6.97
	GPF	60.89 \pm 0.71	66.72 \pm 0.84
	GPF-plus	61.39 \pm 0.22	<u>67.58\pm0.67</u>
	EdgePrompt	61.09 \pm 1.22	<u>66.94\pm0.97</u>
	EdgePrompt+	64.66\pm2.20	72.75\pm2.12

Table 8: Accuracy on 5-shot node classification tasks over three datasets. The best-performing method is **bolded**.

Pre-training Strategies	Tuning Methods	Cora	CiteSeer	Pubmed
GraphCL	EdgePrompt (first layer)	57.74 \pm 4.42	42.41 \pm 3.21	67.33 \pm 3.57
	EdgePrompt	58.60 \pm 4.46	43.31 \pm 3.23	67.76\pm3.01
	EdgePrompt+ (first layer)	61.66 \pm 6.81	44.96 \pm 2.63	67.54 \pm 3.95
	EdgePrompt+	62.88\pm6.43	46.20\pm0.99	67.41 \pm 5.25
EP-GPPT	EdgePrompt (first layer)	36.74 \pm 4.79	29.47 \pm 3.16	47.98 \pm 6.42
	EdgePrompt	37.26 \pm 4.53	29.83 \pm 1.01	47.20 \pm 7.06
	EdgePrompt+ (first layer)	56.10 \pm 6.39	42.10 \pm 1.41	60.61 \pm 7.57
	EdgePrompt+	56.41\pm3.62	43.49\pm2.62	61.51\pm4.91

Table 9: Accuracy on 50-shot graph classification tasks over three datasets. The best-performing method is **bolded**.

Pre-training Strategies	Tuning Methods	ENZYMES	NCI1	NCI109
SimGRACE	EdgePrompt (first layer)	28.83 \pm 1.74	61.58 \pm 2.71	61.82 \pm 1.15
	EdgePrompt	29.33 \pm 2.30	62.02 \pm 3.02	62.02 \pm 1.03
	EdgePrompt+ (first layer)	28.58 \pm 2.45	61.81 \pm 3.03	62.36 \pm 0.98
	EdgePrompt+	32.67\pm2.53	67.07\pm1.96	66.53\pm1.30
EP-GraphPrompt	EdgePrompt (first layer)	30.75 \pm 1.03	61.81 \pm 2.57	62.07 \pm 1.42
	EdgePrompt	30.80 \pm 2.09	61.75 \pm 2.49	62.33 \pm 1.65
	EdgePrompt+ (first layer)	31.92 \pm 1.41	62.07 \pm 2.64	61.66 \pm 1.64
	EdgePrompt+	33.27\pm2.71	65.06\pm1.84	64.64\pm1.57

D.4 MORE RESULTS ON CONVERGENCE PERFORMANCE

Figure 5 illustrates the accuracy curves of our method and the baselines under two pre-training strategies for graph classification.

D.5 RESULTS WITH DIFFERENT SHOTS

We conduct experiments with different shots. Table 10 shows the performance for 10-shot node classification tasks. In addition, we also conduct experiments for 100-shot graph classification tasks

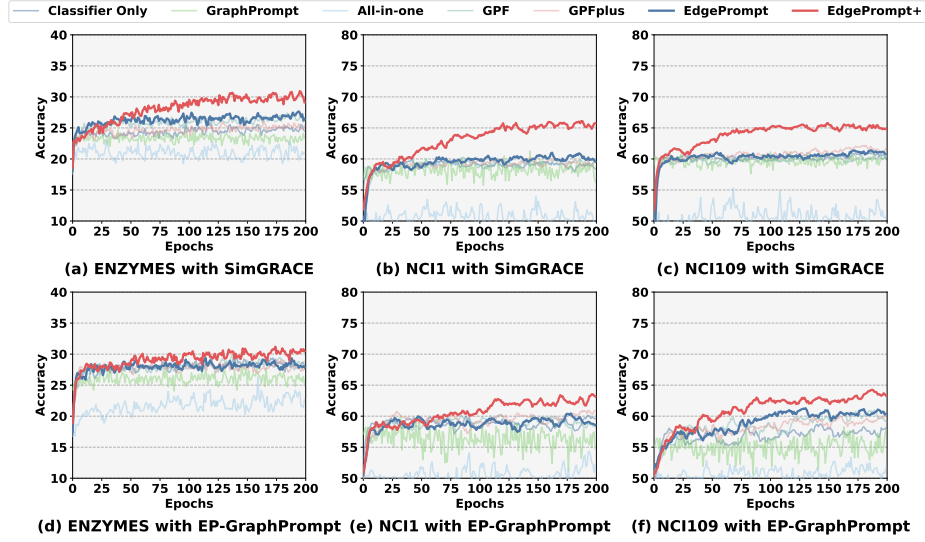


Figure 5: Convergence speeds of different methods.

and report the results in Table 11. Since ENZYMES uses up all graphs as the training samples in the 100-shot setting, we run experiments on the remaining four datasets.

E FUTURE WORKS

In the future, we will investigate the performance of our method under more pre-training strategies, such as DGI (Veličković et al., 2019), InfoGraph (Sun et al., 2020), GraphMAE (Hou et al., 2022). In addition, we will explore other designs for edge prompts, such as conditional prompting Yu et al. (2024c); Zhou et al. (2022). Furthermore, we will also study how to adapt our method for heterogeneous graphs.

Table 10: Accuracy on 10-shot node classification tasks over five datasets. The best-performing method is **bolded** and the runner-up is underlined.

Pre-training Strategies	Tuning Methods	Cora	CiteSeer	Pubmed	ogbn-arxiv	Flickr
GraphCL	Classifier Only	65.43 \pm 2.29	43.97 \pm 4.39	68.23 \pm 1.05	26.78 \pm 1.66	30.34 \pm 2.33
	GPPT	58.38 \pm 3.43	44.65 \pm 8.47	67.71 \pm 6.35	26.54 \pm 3.69	28.80 \pm 5.93
	GraphPrompt	63.55 \pm 2.49	46.17 \pm 3.07	67.73 \pm 1.83	25.51 \pm 1.00	26.74 \pm 1.90
	ALL-in-one	51.57 \pm 7.11	43.31 \pm 2.78	61.20 \pm 2.83	21.84 \pm 2.45	24.63 \pm 3.75
	GPF	70.06 \pm 1.88	47.34 \pm 4.22	70.70 \pm 1.30	27.43 \pm 1.51	27.59 \pm 2.21
	GPF-plus	65.32 \pm 1.93	43.97 \pm 3.97	68.32 \pm 0.91	26.75 \pm 1.32	29.81 \pm 1.43
	EdgePrompt	70.20 \pm 1.77	47.85 \pm 4.19	70.54 \pm 1.55	27.52 \pm 1.20	28.58 \pm 2.50
	EdgePrompt+	74.27\pm3.46	52.93\pm4.20	72.70\pm2.50	28.79\pm1.21	30.74\pm2.30
SimGRACE	Classifier Only	62.18 \pm 3.15	45.62 \pm 3.74	60.60 \pm 1.87	27.09 \pm 0.93	30.35 \pm 1.90
	GPPT	60.00 \pm 5.11	40.27 \pm 7.11	62.16 \pm 6.35	27.26 \pm 3.44	30.31 \pm 6.39
	GraphPrompt	59.26 \pm 2.06	47.22 \pm 3.37	62.53 \pm 1.71	25.66 \pm 0.83	30.16 \pm 1.22
	ALL-in-one	49.83 \pm 2.90	43.94 \pm 2.83	59.99 \pm 1.99	20.03 \pm 3.03	29.64 \pm 3.72
	GPF	67.73 \pm 4.06	49.08 \pm 3.36	63.58 \pm 1.65	27.92 \pm 0.94	32.96 \pm 3.94
	GPF-plus	62.22 \pm 3.36	45.44 \pm 4.15	60.67 \pm 1.77	27.09 \pm 0.82	33.89\pm3.31
	EdgePrompt	68.28 \pm 4.05	49.29 \pm 3.45	63.67 \pm 1.66	27.88 \pm 1.00	33.56 \pm 3.58
	EdgePrompt+	72.57\pm3.50	52.78\pm3.29	69.56\pm2.58	28.70\pm0.91	32.17 \pm 2.77
EP-GPPT	Classifier Only	34.12 \pm 3.25	28.42 \pm 3.32	45.05 \pm 4.12	15.94 \pm 1.80	31.96 \pm 5.48
	GPPT	48.43 \pm 6.16	35.94 \pm 6.09	56.50 \pm 9.44	23.58\pm1.84	29.58 \pm 6.81
	GraphPrompt	35.08 \pm 1.43	28.12 \pm 1.56	48.71 \pm 5.28	13.38 \pm 1.84	29.08 \pm 3.51
	ALL-in-one	35.12 \pm 1.62	27.19 \pm 2.63	47.11 \pm 1.56	16.57 \pm 0.37	32.30\pm2.42
	GPF	49.61 \pm 0.40	35.19 \pm 2.46	50.52 \pm 2.75	22.48 \pm 2.21	31.60 \pm 5.54
	GPF-plus	33.60 \pm 2.34	28.18 \pm 3.31	45.13 \pm 4.67	16.07 \pm 1.82	30.81 \pm 7.60
	EdgePrompt	50.43 \pm 0.83	34.56 \pm 3.04	50.90 \pm 2.51	22.61 \pm 2.21	30.80 \pm 6.58
	EdgePrompt+	69.65\pm6.44	50.74\pm2.80	60.83\pm4.36	21.66 \pm 2.06	30.78 \pm 5.75
EP-GraphPrompt	Classifier Only	68.17 \pm 3.25	47.94 \pm 3.58	75.49 \pm 1.79	36.69 \pm 0.80	31.38 \pm 8.08
	GPPT	68.93 \pm 4.55	48.83 \pm 8.45	74.78 \pm 6.81	25.65 \pm 3.55	32.85 \pm 3.09
	GraphPrompt	68.95 \pm 2.57	50.26 \pm 2.21	75.73 \pm 1.40	36.86 \pm 0.84	30.39 \pm 5.31
	ALL-in-one	57.74 \pm 3.19	46.14 \pm 5.72	74.24 \pm 3.04	22.84 \pm 2.60	30.61 \pm 5.28
	GPF	<u>72.24\pm2.92</u>	51.07 \pm 3.76	77.77\pm2.42	36.91 \pm 1.09	29.74 \pm 8.94
	GPF-plus	68.32 \pm 3.75	48.33 \pm 3.62	75.57 \pm 1.73	36.63 \pm 1.08	29.40 \pm 8.30
	EdgePrompt	72.20 \pm 2.47	51.40 \pm 3.60	<u>77.35\pm2.52</u>	<u>37.16\pm1.18</u>	32.01 \pm 4.61
	EdgePrompt+	75.08\pm3.11	56.09\pm2.63	76.66 \pm 2.07	37.28\pm1.43	34.49\pm7.10

Table 11: Accuracy on 100-shot graph classification tasks over four datasets. The best-performing method is **bolded** and the runner-up underlined.

Pre-training Strategies	Tuning Methods	DD	NCI1	NCI109	Mutagenicity
GraphCL	Classifier Only	63.23 \pm 1.42	62.03 \pm 1.60	62.18 \pm 1.59	68.29 \pm 1.26
	GraphPrompt	62.80 \pm 1.15	62.17 \pm 1.21	61.79 \pm 0.99	68.14 \pm 0.94
	All-in-one	66.33 \pm 1.78	60.69 \pm 1.15	62.00 \pm 0.37	64.39 \pm 2.74
	GPF	66.75 \pm 1.14	62.48 \pm 1.65	61.98 \pm 0.97	68.41 \pm 1.60
	GPF-plus	68.49\pm1.98	65.39 \pm 2.27	64.85 \pm 1.41	68.78 \pm 1.22
	EdgePrompt	66.96 \pm 1.05	63.84 \pm 1.75	62.42 \pm 0.91	68.69 \pm 1.59
	EdgePrompt+	67.81 \pm 1.49	67.54\pm1.40	67.94\pm0.81	70.52\pm0.58
SimGRACE	Classifier Only	63.74 \pm 0.96	63.27 \pm 1.68	63.20 \pm 2.00	67.65 \pm 1.28
	GraphPrompt	63.82 \pm 0.95	63.58 \pm 1.35	61.52 \pm 1.10	67.97 \pm 0.97
	All-in-one	68.92\pm0.61	59.94 \pm 2.12	62.79 \pm 0.48	64.47 \pm 2.02
	GPF	65.90 \pm 2.02	64.32 \pm 1.55	63.48 \pm 1.82	67.44 \pm 1.01
	GPF-plus	67.04 \pm 1.53	65.28 \pm 2.05	64.72 \pm 1.64	67.95 \pm 0.88
	EdgePrompt	65.99 \pm 2.29	65.09 \pm 1.46	63.65 \pm 1.69	68.23 \pm 0.81
	EdgePrompt+	68.03 \pm 1.85	67.24\pm1.87	67.59\pm1.63	69.50\pm0.54
EP-GPPT	Classifier Only	62.68 \pm 1.93	58.47 \pm 1.07	63.24 \pm 0.67	66.57 \pm 1.26
	GraphPrompt	60.55 \pm 1.53	59.11 \pm 0.66	62.76 \pm 0.85	67.12 \pm 1.42
	All-in-one	62.51 \pm 1.25	59.06 \pm 1.47	62.07 \pm 0.96	65.04 \pm 0.84
	GPF	63.82 \pm 3.44	59.31 \pm 1.49	63.75 \pm 0.63	66.64 \pm 1.34
	GPF-plus	68.87\pm2.80	64.48 \pm 2.57	65.10 \pm 0.81	69.00 \pm 1.10
	EdgePrompt	64.84 \pm 3.27	60.57 \pm 1.57	63.60 \pm 0.67	67.15 \pm 1.40
	EdgePrompt+	68.28 \pm 2.03	66.28\pm1.15	66.72\pm1.34	71.52\pm1.58
EP-GraphPrompt	Classifier Only	65.95 \pm 1.79	62.88 \pm 0.81	62.02 \pm 2.27	67.39 \pm 0.80
	GraphPrompt	66.24 \pm 1.70	62.93 \pm 0.97	62.27 \pm 1.05	67.67 \pm 0.74
	All-in-one	66.45 \pm 1.24	60.73 \pm 1.46	58.56 \pm 0.70	66.53 \pm 1.10
	GPF	68.37 \pm 2.66	62.68 \pm 1.45	63.75 \pm 1.67	67.98 \pm 0.97
	GPF-plus	68.89 \pm 3.93	63.91 \pm 0.99	63.55 \pm 2.42	67.84 \pm 0.96
	EdgePrompt	67.81 \pm 3.64	63.33 \pm 1.40	64.00 \pm 1.91	68.04 \pm 1.07
	EdgePrompt+	69.04\pm2.96	66.80\pm0.55	65.94\pm1.15	71.48\pm1.89