Can Graph Neural Networks Learn Language with Extremely Weak Text Supervision?

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Abstract

While great success has been achieved in building vision models with Contrastive Language-Image Pre-training (CLIP) over internet-scale image-text pairs, building transferable Graph Neural Networks (GNNs) with CLIP pipeline is challenging because of the scarcity of labeled data and text supervision, different levels of downstream tasks, and the conceptual gaps between domains. In this work, to address these issues, we propose a multi-modal prompt learning paradigm to effectively adapt pre-trained GNN to downstream tasks and data, given only a few semantically labeled samples, each with extremely weak text supervision. Our new paradigm embeds the graphs directly in the same space as the Large Language Models (LLMs) by learning both graph prompts and text prompts simultaneously. We demonstrate the superior performance of our paradigm in few-shot, multi-task-level, and cross-domain settings. Moreover, we build the first CLIP-style zero-shot classification prototype that can generalize GNNs to unseen classes with extremely weak text supervision. The code is available at https://github.com/Violet24K/Morpher.

1 Introduction

Graphs are constructed from real scenarios, but GNNs, optimized according to numerical labels, still do not *understand* what a label represents in the real world. To solve the issue of predetermined numerical categories, CLIP (Radford et al., 2021) leverages natural language supervision by jointly training an image encoder and a text encoder in the same embedding space at scale. CLIP has demonstrated the ability to train high-quality, generalizable vision models (Radford et al., 2021; Jia et al., 2021; Li et al., 2022), which can adapt to diverse downstream tasks. Similar frameworks have been successfully extended to video (Xu et al., 2021), 3D images (Hess et al., 2024), speech (Shih et al., 2022) and audio (Guzhov et al., 2022), consistently demonstrating that alignment with text enhances the transferability of encoders. As for graphs, so far, such graph-text alignment has only been explored in the molecular domain (Luo et al., 2023; Liu et al., 2023e) and on text-attributed graphs (Wen and Fang, 2023; Li et al., 2023a; Jin et al., 2023b; Yan et al., 2023), where the paired graph-text data is relatively sufficient for joint pre-training.

However, extending this paradigm to more general graph data poses significant challenges due to three facts. First, compared with language or vision data, graph data is very scarce and the text supervision is extremely weak (Liu et al., 2023a; Chen et al., 2023b; Manchanda et al., 2023). Besides the number of samples being much smaller than images, many graph datasets are used for classification, where the label names consist of only a few tokens. Second, the task space of graph data could be on node-level, edge-level, and graph-level. Third, in general, language tokens and visual objects retain the same conceptual meaning across different distributions, but the same graph structure may have distinct interpretations in different domains.

Jointly pre-training graph and text encoders is impractical for graph data with extremely weak text supervision. Fortunately, we can deal with the two modalities separately for pre-training: large language models have already been extensively pre-trained, and tremendous efforts have been devoted to pre-train GNNs through self-supervision (Hu et al., 2020a; Liu et al., 2023c; Zheng et al., 2024c,d). However, even with a pre-trained graph model, effectively adapting it to both the semantic embedding space for text alignment and diverse downstream tasks remains non-trivial. This raises a critical question:

How to adapt pre-trained GNNs to the semantic embedding space given limited downstream data,

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i.e., few samples and weak text supervision?

This paper aims to answer this question based on the following observations: (1) Semantic text embedding spaces do not necessarily result from joint pre-training. In fact, the embedding spaces of encoder LLMs are inherently semantic and high-quality, as LLMs are trained on massive text data and demonstrate strong performances. (2) When the downstream data are limited, prompt learning (Li and Liang, 2021; Houlsby et al., 2019; Zhang et al., 2022a; Lester et al., 2021) provides a better option than fine-tuning as much fewer parameters not only makes the optimization more efficient but also requires less resource than fine-tuning a large model. Notably, some works have explored prompt learning for better alignment and obtained improvement in vision prediction (Zhou et al., 2022b; Khattak et al., 2023). Inspired by these observations, we propose a prompting-based paradigm with an LLM that aligns the GNN representations in the semantic embedding space, while keeping the parameters of both GNN and LLM frozen.

When adapting the representation from one modality to another, solely prompting a single modality could be sub-optimal, as it limits the adjustment to downstream tasks in the other modality (Khattak et al., 2023). To this end, we propose Multi-modal Prompt Learning for Graph Neural Networks (Morpher). Given a pre-trained GNN and few-shot semantically labeled graph data with weak text supervision, we assume zeroth-order access to a pre-trained LLM. Then, to leverage its high-quality semantic embedding space, Morpher connects and aligns the graph embeddings to it through prompting on both modalities with a cross-modal projector. Nonetheless, designing such a paradigm is more challenging than vision-language models. First, we lack jointly pre-trained encoders for the two modalities; instead, we only have two encoders pre-trained independently in each modality. Second, determining how to prompt the graph modality is non-trivial and remains a trending research topic. Third, the downstream data for GNN usually have much fewer labeled classes and labeled samples than Vision-Language models, and the text supervision is extremely weak. Our contributions towards tackling these challenges are:

- We analyze that, state-of-the-art graph prompt (Sun et al., 2023a) is often unable to learn good representations of the downstream data. We further improve it to prevent unstable optimization.
- To connect and adapt the pre-trained GNN with LLM effectively with extremely weak text supervision, we propose Morpher, the first graph-text multi-modal prompt learning paradigm to align the representations of GNN and LLM without fine-tuning any of their parameters.
- With extremely weak text supervision, we demonstrate our improved graph prompt and Morpher under few-shot, multi-task, and cross-domain settings. To show that GNN learns language dependency through Morpher, we present the first CLIP-style zero-shot generalization prototype where the GNN can predict unseen classes.

2 Background

We use calligraphic letters (e.g., $\mathcal{A}$) for sets, and specifically $\mathcal{G}$ for graphs. We use bold capital letters for matrices (e.g., $\mathbf{A}$). For matrix indices, we use $\mathbf{A}(i,j)$ to denote the entry in the i^{th} row and the j^{th} column. $\mathbf{A}(i,:)$ is the i^{th} row in $\mathbf{A}$.

Graph Neural Networks. We use $\mathcal{G} = (\mathbf{A}, \mathbf{X})$ to denote a graph with node set $\mathcal{V}$ and edge set $\mathcal{E}$, where $\mathbf{A} \in \mathbb{R}^{|\mathcal{V}|\times|\mathcal{V}|}$ is the adjacency matrix and $\mathbf{X} \in \mathbb{R}^{|\mathcal{V}|\times d}$ is the node feature matrix. $\mathbf{A}(u,v) = 1$ if there is an edge connecting u and v; otherwise $\mathbf{A}(u,v) = 0$. A graph neural network $f_\phi^g(\cdot)$ with hidden dimension d_g encodes $\mathcal{G}$ into the embedding space: $f_\phi^g(\mathcal{G}) \in \mathbb{R}^{|\mathcal{V}|\times d_g}$, which could preserve both feature and structure information of $\mathcal{G}$.

Few-shot Prompt Learning. Let $f_\phi^t(\cdot)$ denote the LLM encoder with embedding dimension d_t. For a series of input tokens $\{x_k\}_{k=1}^K$, the LLM encoder embeds it as a matrix $\mathbf{X}_t = f_\phi^t(\{x_k\}_{k=1}^K) \in \mathbb{R}^{K\times d_t}$. Prompt learning initializes a tunable matrix $\mathbf{P}_\theta^t \in \mathbb{R}^{n_t\times d_t}$, where n_t denotes the number of text prompt tokens. Then, this tunable matrix is concatenated with the input tokens' embeddings to form $[\mathbf{P}_\theta^t; \mathbf{X}_t]_{dim=0} \in \mathbb{R}^{(K+n_t)\times d_t}$.

Our Problem Set-up. Given a pre-trained GNN $f_\phi^g(\cdot)$ with embedding dimension d_g and a pre-trained LLM encoder $f_\phi^t(\cdot)$ with embedding dimension d_t. Without loss of generality, we assume the downstream task is graph-level classification, as node-level or edge-level GNN tasks can be reformulated as graph-level by inducing ego-graphs within neighbor distance γ. For L-shot graph classification, we are given limited text-labeled pairs $\{(\mathcal{G}_i, t_c)\}_{i=1}^L$ for each class c. Each text label t_c consists of only a few tokens. Assuming $\mathcal{T}$ is the

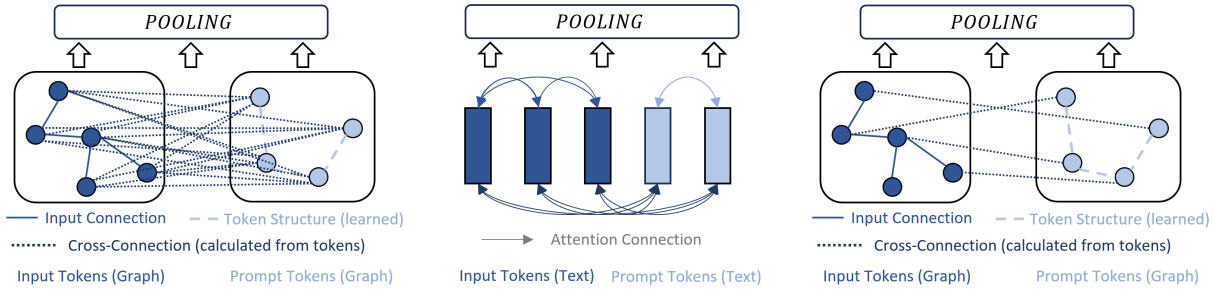

Figure 1: Cross-connections overwhelm inner-connections in current graph prompt design, which may be unstable during training (left); attention in NLP where $3 \times 2 = 6$ cross-connections and $3 + 1 = 4$ inner-connections are balanced (middle); and our balanced graph prompt design (right). **The cross-connections between input and prompt should have a consistent scale with the input connections.**

set of all text labels t_c, we are provided a set of test graphs $\{\mathcal{G}_j\}_{j=1}^{L_{test}}$ and want to predict the text label $t_j \in \mathcal{T}$ for each test graph $\mathcal{G}_j$.

3 Improving Single-modal Graph Prompt

Unlike prompting text data, prompting graph data presents a significant challenge due to the non-euclidean nature of graphs. The pioneering work (Sun et al., 2023a) designs the graph prompt still as a graph and then inserts it into the original graph.

Current Graph Prompt Design. To prompt a graph $\mathcal{G}$, each prompt token is a new node. Let n_g denote the number of prompt tokens and $\mathcal{P} = \{p_i\}_{i=1}^{n_g}$ denote the set of prompt tokens. The graph prompt is formulated by a tunable matrix $\mathbf{P}_\theta^g \in \mathbb{R}^{n_g \times d}$, where d is the node feature dimension. Each row vector $\mathbf{P}_\theta^g(i,:)$ is the feature of the prompt token p_i. Then, the mechanism to prompt a graph $\mathcal{G} = (\mathbf{A}, \mathbf{X})$ with n nodes and d feature dimension is (Sun et al., 2023a)

- Compute inner-connections to construct the prompt graph $\mathcal{G}_p = (\mathbf{A}_p, \mathbf{X}_p) = (\mathbf{A}_p, \mathbf{P}_\theta^g)$. For two prompt tokens p_i and p_j, $\mathbf{A}_p(i,j) = 1 \iff \sigma(\mathbf{P}_\theta^g(i,:)\mathbf{P}_\theta^g(j,:)^\top) > \delta_{inner}$, where $\sigma(\cdot)$ is the sigmoid function.

- Compute cross-connections to insert the prompt graph $\mathcal{G}_p$ into $\mathcal{G}$. Similarly, for $x_i \in \mathcal{G}$ and $p_j \in \mathcal{G}_p$, there is an edge between them if and only if $\sigma(\mathbf{X}(i,:)\mathbf{P}_\theta^g(j,:)^\top) > \delta_{cross}$.

- Construct the prompted graph (i.e., manipulated graph) $\mathcal{G}_m = (\mathbf{A}_m, \mathbf{X}_m)$. The overall adjacency matrix $\mathbf{A}_m \in \mathbb{R}^{(n+n_g)\times(n+n_g)}$ is constructed from the original adjacency matrix $\mathbf{A}$, the inner edges $\mathbf{A}_p$ and the cross edges. The overall node feature matrix is concatenated from the prompt token features and the original input node features: $\mathbf{X}_m = [\mathbf{P}_\theta^g; \mathbf{X}]_{dim=0} \in \mathbb{R}^{(n+n_g)\times d}$.

Issues associated with the current design. The input node features of most real-world datasets are sparse, resulting from the construction process (Yang et al., 2016; Morris et al., 2020; Dwivedi et al., 2023). As shown in Appendix Table 4, $||\mathbf{X}(i,:)||_1$ is typically 1. As the initialization of each token feature tensor $\mathbf{P}_\theta^g(i,:)$ is close to $\vec{\mathbf{0}}$ to stabilize gradients, for any node i and token p_j, the dot products $\mathbf{X}(i,:)\mathbf{P}_\theta^g(j,:)^\top$ is close to 0, and the sigmoid value is very close to 0.5. Consequently, if we want the graph prompt to have cross-connections, we must set $\delta_{cross} < 0.5$. Then, as the sigmoid values are close to 0.5, the cross-connections will be dense, i.e., almost every node in the original graph is connected with every node token in the prompt graph. For two different graphs $\mathcal{G}_1$ and $\mathcal{G}_2$ in the same task, the prompt graph $\mathcal{G}_p$ is identical. Since the GNNs aggregate the node features, their embeddings $f_\phi^g(\mathcal{G}_1)$ and $f_\phi^g(\mathcal{G}_2)$ are approximately the same because the features in the prompt graph overwhelm the features in the original graphs due to the dense cross-connections. Then, even if $\mathcal{G}_1$ and $\mathcal{G}_2$ have different labels, the task head classifier cannot be trained to distinguish them [1].

In Appendix C.1, we show that initializing graph prompt token feature tensor with higher variance cannot effectively address this problem.

Improved Graph Prompt Design. The issue of the current graph prompt lies in the significant imbalance between original connections within the input graph and the input-prompt cross-connections, as illustrated in Figure 1 (left). We also visualize

[1] In fact, similar training instability problems have been observed by another work (Zhao et al., 2024).

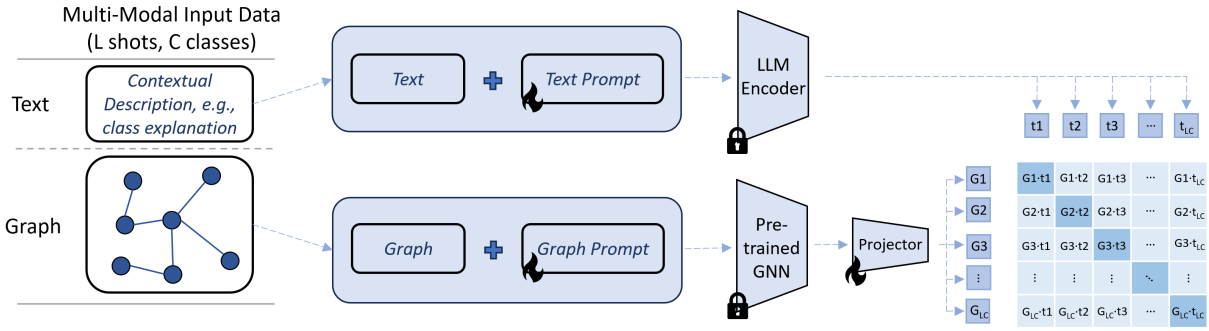

Figure 2: Similar to CLIP backbone, Morpher adapts the graph representations to semantic space through multi-modal prompt learning, even if the GNN and LLM are not jointly trained and are kept frozen.

the standard NLP attention mechanism (Vaswani et al., 2017) in Figure 1 (middle). When a sequence of text prompt tokens p_i^t is prepended to the input sequence, the features of the prompt tokens will be aggregated with those of the input tokens through a dense "cross-connection", i.e., attention. Simultaneously, the features within the input sequence are also densely aggregated via attention, maintaining a balance with the prompt-input aggregation to prevent overwhelming. Inspired by this, we deem that a balance could be achieved by approximately equalizing the number of cross-connections with that of input graph connections, i.e., n_e. Since the connection of a graph dataset is often sparse, we constrain the cross-connections to be sparse as well. Therefore, we set the number of cross-connections to at most n_e by connecting each node in the input graph with at most $\lfloor \frac{n_e}{a} \rfloor$ prompt tokens. Then, we can safely use a small δ_{cross} and cosine similarity $\frac{\mathbf{X}(i,:)\cdot\mathbf{P}_\theta^g(j,:)^\top}{\|\mathbf{X}(i,:)\|_2\|\mathbf{P}_\theta^g(j,:)\|_2}$ instead of $\sigma(\mathbf{X}(i,:)\mathbf{P}_\theta^g(j,:)^\top)$ to calculate the cross-connections.

4 GNN Multi-modal Prompt Learning

To adapt the GNN embeddings to the LLM's semantic embedding space and leverage the additional weak supervision provided by the text associated with graph labels, we explore the potential of multi-modal prompt learning for both graphs and language. This approach is motivated by the intuition that only prompting on the graph data may limit the flexibility to adjust the LLM representation space. The overall paradigm of Morpher is illustrated in Figure 2. Given the data $\{(\mathcal{G}_i, t_i)\}_{i=1}^{L\times C}$, we aim to align graph embedding $\text{readout}(f_\phi^g(\mathcal{G}_i))$ with $\text{readout}(f_\phi^t(\text{Tokenize}(t_i)))$. Yet one direct issue is that, $\text{readout}(f_\phi^g(\mathcal{G}_i)) \in \mathbb{R}^{1\times d_g}$ and $\text{readout}(f_\phi^t(\text{Tokenize}(t_i))) \in \mathbb{R}^{1\times d_t}$ may have distinct dimensions. To address this issue, we adopt a cross-modal projector that learns to map the graph embedding space to the text embedding space. For an input d_g-dimensional graph embedding $\mathbf{v}$, the projector maps it to a vector $\widetilde{\mathbf{v}}$ in the d_t-dimensional text embedding space:

$$\widetilde{\mathbf{v}} = \text{Proj}_\theta(\mathbf{v}) := \tanh(\mathbf{W}\mathbf{v} + \mathbf{b}) \in \mathbb{R}^{1\times d_t} \quad (1)$$

As discussed in Sections 2 and 3, we introduce the text prompt $\mathbf{P}_\theta^t \in \mathbb{R}^{n_t\times d_t}$ with n_t text prompt tokens and the graph prompt $\mathbf{P}_\theta^g \in \mathbb{R}^{n_g\times d}$ with n_g graph prompt tokens. The graph prompting function $\psi_g(\cdot, \mathbf{P}_\theta^g)$ modifies a given graph $\mathcal{G}$ into a manipulated graph $\mathcal{G}m = \psi_g(\mathcal{G}, \mathbf{P}_\theta^g)$.

Let $\omega_t(\cdot, \mathbf{P}_\theta^t)$ be the prompted text embedding given input text t. For the text prompt methods we choose, the prompted embedding is

$$\omega_t(t, \mathbf{P}_\theta^t) = [\mathbf{P}_\theta^t; f_\phi^t(\text{Tokenize}(t))]_{dim=0} \quad (2)$$

Let $\omega_g(\cdot, \mathbf{P}_\theta^g)$ be the prompted graph embedding given input graph $\mathcal{G}$, then we have:

$$\omega_g(\mathcal{G}, \mathbf{P}_\theta^g) = f_\phi^g(\mathcal{G}_m) = f_\phi^g(\psi_g(\mathcal{G}, \mathbf{P}_\theta^g)) \quad (3)$$

For the whole prompted text and the whole prompted graph of the sample $(\mathcal{G}_i, t_i)$, we apply readout (e.g., mean-pooling, max-pooling, etc.) to get their embedding:

$$\mathbf{h}_i^t = \text{readout}(\omega_t(t_i, \mathbf{P}_\theta^t)) \in \mathbb{R}^{1\times d_t} \quad (4)$$

$$\mathbf{h}_i^\mathcal{G} = \text{readout}(\omega_g(\mathcal{G}_i, \mathbf{P}_\theta^g)) \in \mathbb{R}^{1\times d_g} \quad (5)$$

For the given data $(\mathcal{G}_i, t_i)$, we compute the normalized embedding of prompted $\mathcal{G}_i$ and project it to the text embedding space through the projector:

$$\mathbf{z}_{norm,i}^\mathcal{G} = \frac{\mathbf{h}_i^\mathcal{G}}{||\mathbf{h}_i^\mathcal{G}||_2} = \frac{\text{readout}(\omega_g(\mathcal{G}_i, \mathbf{P}_\theta^g))}{||\text{readout}(\omega_g(\mathcal{G}_i, \mathbf{P}_\theta^g))||_2} \quad (6)$$

$$\mathbf{z}_i^\mathcal{G} = \text{Proj}_\theta(\mathbf{z}_{norm,i}^\mathcal{G}) \quad (7)$$

For the text embeddings, since for limited data the set $\mathcal{T} = \{t_i\}_{i=1}^{C}$ may contain texts that are semantically close as discussed in Appendix A.2, we extract a subspace in the text embedding space by normalizing the embedding as follows. We further normalize the text embeddings to the unit sphere.

$$\mu = \frac{1}{L}\sum_{i=1}^{L}\mathbf{h}_i^t, \quad \mathbf{h}_{norm,i}^t = \mathbf{h}_i^t - \mu \tag{8}$$

$$\mathbf{z}_i^t = \frac{\mathbf{h}_{norm,i}^t}{||\mathbf{h}_{norm,i}^t||_2} = \frac{\text{readout}(\omega_t(t_i, \mathbf{P}_\theta^t)) - \mu}{||\text{readout}(\omega_t(t_i, \mathbf{P}_\theta^t)) - \mu||_2} \tag{9}$$

Finally, we use the in-batch similarity-based contrastive loss with temperature τ to train text prompts, graph prompts, and the projector.

$$\mathcal{L}_{G\to T} = -\frac{1}{B}\sum_{i=1}^{B}\log\frac{\exp(\mathbf{z}_i^{\mathcal{G}}\cdot\mathbf{z}_i^t/\tau)}{\sum_{j=1}^{B}\exp(\mathbf{z}_i^{\mathcal{G}}\cdot\mathbf{z}_j^t/\tau)} \tag{10}$$

During inference stage, for an input graph $\mathcal{G}_i$ and text label candidates $\mathcal{T} = \{t_i\}_{i=1}^{C}$, we compute the embedding $\mathbf{z}_i^{\mathcal{G}} = \text{Proj}_\theta(\frac{\text{readout}(\omega_g(\mathcal{G}_i, \mathbf{P}_\theta^g))}{||\text{readout}(\omega_g(\mathcal{G}_i, \mathbf{P}_\theta^g))||_2})$ using trained $\mathbf{P}_\theta^g$ and $\text{Proj}_\theta(\cdot)$. Then, we compute $\mathbf{z}_i^t$ as Equations 9 and 10. Finally, $\mathcal{G}_i$ will be classified to associate with text label $\arg\max_{1\le i\le C}(\mathbf{z}_i^{\mathcal{G}}\cdot\mathbf{z}_i^t)$.

5 Experiments

We show that both Morpher and the improved graph prompt more effectively adapt pre-trained GNNs to the specific downstream classification task. We use RoBERTa (Liu et al., 2019) as the LLM encoder for Morpher in the main experiments. We also validate the performance of Morpher with ELECTRA (Clark et al., 2020) and DistilBERT (Sanh et al., 2019) in Appendix B.3.

Datasets. We use real-world graph datasets from PyTorch Geometric (Fey and Lenssen, 2019), including one molecular dataset MUTAG (Morris et al., 2020); two bioinformatic datasets ENZYMES and PROTEINS (Borgwardt et al., 2005); one computer vision dataset MSRC_21C (Neumann et al., 2016); three citation network datasets Cora, CiteSeer and PubMed (Yang et al., 2016). We use real-world class names as text labels. The text supervision is extremely weak, as each text label contains no more than five words. More details are summarized in Appendix A.

Pre-training algorithms and GNN backbones. To pretrain GNNs for evaluation, we adopt GraphCL (You et al., 2020) and SimGRACE (Xia et al., 2022) to pre-train three widely used GNN backbones: GCN (Kipf and Welling, 2016), GAT (Yun et al., 2019) and GraphTransformer (GT) (Khosla et al., 2020). Additionally, in Appendix B.4, we verify the effectiveness of our methods on GNNs pre-trained using GraphMAE (Hou et al., 2022) and MVGRL (Hassani and Ahmadi, 2020), two other representative GNN self-supervised learning algorithms. For each dataset, to pre-train GNNs, we leverage self-supervised learning methods on all the graphs without any label information.

Baselines. We compare our methods with the following baselines: (1) training a GNN from scratch supervised by few-shot data (*"supervised"*); (2) fine-tuning a task head together with pre-trained GNN (*"fine-tune"*). We allow GNNs to be tunable for "*supervised*" and "*fine-tune*"; (3) state-of-the-art graph prompting algorithms: All-in-one (*"AIO"*) (Sun et al., 2023a), which is the only graph prompting algorithm that supports multiple tasks in node-level, edge-level and graph-level to the best of our knowledge; GPF-plus (Fang et al., 2023) which prompt on graph features and Gprompt (Liu et al., 2023d) which is based on subgraph similarity.

5.1 Few-shot Learning

We investigate our improved graph prompt ("*ImprovedAIO*") and Multimodal prompt ("*Morpher*") to adapt frozen pre-trained GNNs using few-shot data. We focus on graph-level classification here and will further investigate the few-shot learning ability at other task levels in Section 5.2. Our few-shot learning setting is more challenging than existing works (Sun et al., 2023a, 2022) as we only allow no more than 10 labeled training and validation samples for each class. The results are shown in Table 1. By observations, given the same pre-trained GNN, our ImprovedAIO outperforms all the existing baseline methods. This improvement is attributed to its design, which restricts cross-connections, ensuring stable training and optimization. Moreover, Our Morpher can achieve an absolute further accuracy improvement over the baselines across all datasets. Its superior performance, even under extremely weak text supervision, stems from its ability to dynamically adapt and align the graph and language representation spaces with prompt learning. This flexibility enables Morpher to better leverage the semantic information from weakly-supervised text labels while preserving the structural integrity of the graph embeddings, resulting in more robust and accurate predictions.

Training schemes	GNN pretraining	MUTAG Acc	MUTAG F1	ENZYMES Acc	ENZYMES F1	PROTEINS Acc	PROTEINS F1	MSRC_21C Acc	MSRC_21C F1
Supervised	N/A + GCN	66.00	66.67	16.67	8.68	65.89	60.77	38.85	35.32
	N/A + GAT	66.00	65.69	16.45	4.65	64.75	64.08	41.14	39.86
	N/A + GT	66.66	66.26	15.62	4.22	62.81	57.12	38.28	41.62
Pre-train + Fine-tune	GraphCL+GCN	70.00	70.23	17.91	11.82	65.89	61.23	40.00	43.89
	GraphCL+GAT	70.00	69.73	17.91	10.46	65.16	63.92	44.57	45.74
	GraphCL+GT	68.00	67.81	17.70	8.99	63.28	56.41	41.71	43.73
	SimGRACE+GCN	66.67	67.27	17.29	8.78	66.82	64.70	40.57	43.84
	SimGRACE+GAT	70.67	69.10	16.87	7.18	65.42	63.65	42.85	42.37
	SimGRACE+GT	69.33	69.77	16.24	6.08	65.98	62.31	39.42	40.78
AIO (Sun et al., 2023a)	GraphCL+GCN	64.67	39.27	17.50	4.97	61.35	44.93	3.59	10.09
	GraphCL+GAT	64.67	39.27	17.50	4.97	59.21	37.19	14.37	3.11
	GraphCL+GT	73.33	72.06	18.33	9.09	40.79	28.97	17.96	8.30
	SimGRACE+GCN	64.67	39.27	16.04	4.61	67.42	60.87	34.73	18.16
	SimGRACE+GAT	64.67	39.27	16.04	4.61	59.21	37.19	7.78	1.79
	SimGRACE+GT	36.00	27.26	17.50	8.15	50.56	49.34	32.34	15.13
ImprovedAIO (Ours)	GraphCL+GCN	77.33	77.74	18.13	11.98	65.89	65.97	42.85	45.91
	GraphCL+GAT	74.67	75.51	18.33	11.26	65.76	66.05	46.85	51.39
	GraphCL+GT	74.67	74.67	19.16	9.04	68.12	68.18	42.85	43.54
	SimGRACE+GCN	68.00	69.01	17.91	9.02	66.82	66.40	44.57	49.24
	SimGRACE+GAT	77.33	77.20	18.75	9.39	66.91	65.49	45.14	42.31
	SimGRACE+GT	71.33	72.06	18.95	11.25	68.59	68.84	40.57	42.82
Morpher (Ours)	GraphCL+GCN	78.67	78.09	20.41	15.20	67.47	66.40	45.14	49.62
	GraphCL+GAT	**79.33**	**79.15**	**23.12**	**18.01**	70.89	70.30	**50.85**	**54.48**
	GraphCL+GT	76.00	76.51	19.58	13.28	**73.53**	**72.48**	45.71	48.41
	SimGRACE+GCN	69.33	70.27	19.79	14.94	67.10	66.15	45.71	51.24
	SimGRACE+GAT	78.00	77.65	20.21	16.27	68.12	67.26	45.71	51.13
	SimGRACE+GT	74.00	74.84	19.16	14.29	71.76	71.75	44.00	48.16
IMP of ImprovedAIO (%)		3.89 ↑	4.67 ↑	0.90 ↑	1.07 ↑	1.41 ↑	4.64 ↑	2.29 ↑	2.34 ↑
Further IMP of Morpher (%)		2.00 ↑	1.72 ↑	1.84 ↑	5.01 ↑	2.8 ↑	2.24 ↑	2.38 ↑	4.64 ↑

Table 1: Few-shot graph classification performance (%). *IMP (%)*: the average improvement (absolute value) compared to the **best result** among all the baseline methods. Best results are bolded and second-best results are underlined. We also compared with GPF-plus (Fang et al., 2023) and Gprompt (Liu et al., 2023d), in Appendix Table 14 due to space limit.

Tasks	Dataset / Methods	Cora Acc	Cora F1	CiteSeer Acc	CiteSeer F1
Node Level	Supervised	52.83	47.73	63.91	64.82
	Fine-tune	56.37	55.04	64.87	66.42
	AIO (Sun et al., 2023a)	14.69	7.10	18.93	6.92
	ImprovedAIO	58.46	55.10	66.44	66.53
	Morpher	**61.26**	**62.36**	**68.20**	**68.56**
Edge Level	Supervised	51.78	50.62	52.14	50.81
	Fine-tune	52.50	51.00	52.50	51.12
	AIO (Sun et al., 2023a)	50.00	33.33	50.00	33.33
	ImprovedAIO	54.64	54.57	53.92	53.55
	Morpher	**55.71**	**55.05**	**55.35**	**55.05**

Table 2: Node-level, edge-level performance. Best results are bolded and second-best results are underlined.

5.2 Morpher Supports Multiple-level Tasks

Inherited from AIO, our ImprovedAIO and Morpher also support adaptation to downstream tasks at node-level and edge-level, because they can be reformulated into graph-level tasks. After reformulating node classification and task classification as graph classifications by inducing ego-graphs, we use GraphCL+GCN to pre-train the GNN and report the performance in Table 2. The results are consistent with graph level, where ImprovedAIO and Morpher outperform existing methods, with Morpher achieving slightly better performance than ImprovedAIO. Notably, as analyzed in Section 3, AIO is unstable during training, for example in Table 2 (Node level) and in certain cases of Table 1 (e.g., on MSRC_21C with GraphCL or with SimGRACE+GAT). The performance fluctuations observed are consistent and reflect the same underlying issue of AIO. In contrast, our proposed ImprovedAIO effectively addresses this issue.

5.3 Domain Transfer

We explore the potential of using Morpher for domain adaptation. From the previous experiments, we have demonstrated that our ImprovedAIO outperforms the original AIO. Therefore, in the subsequent pages, we focus on comparing Morpher with ImprovedAIO to avoid redundancy. We pre-train GNNs on ENZYMES or CiteSeer datasets, then test the classification performance on MUTAG and PubMed and report the results in Table 3. We unify the pre-train feature dimension with the downstream feature dimension by padding zeros or SVD reduction. From the results, Morpher demonstrates the best transferability, followed by ImprovedAIO.

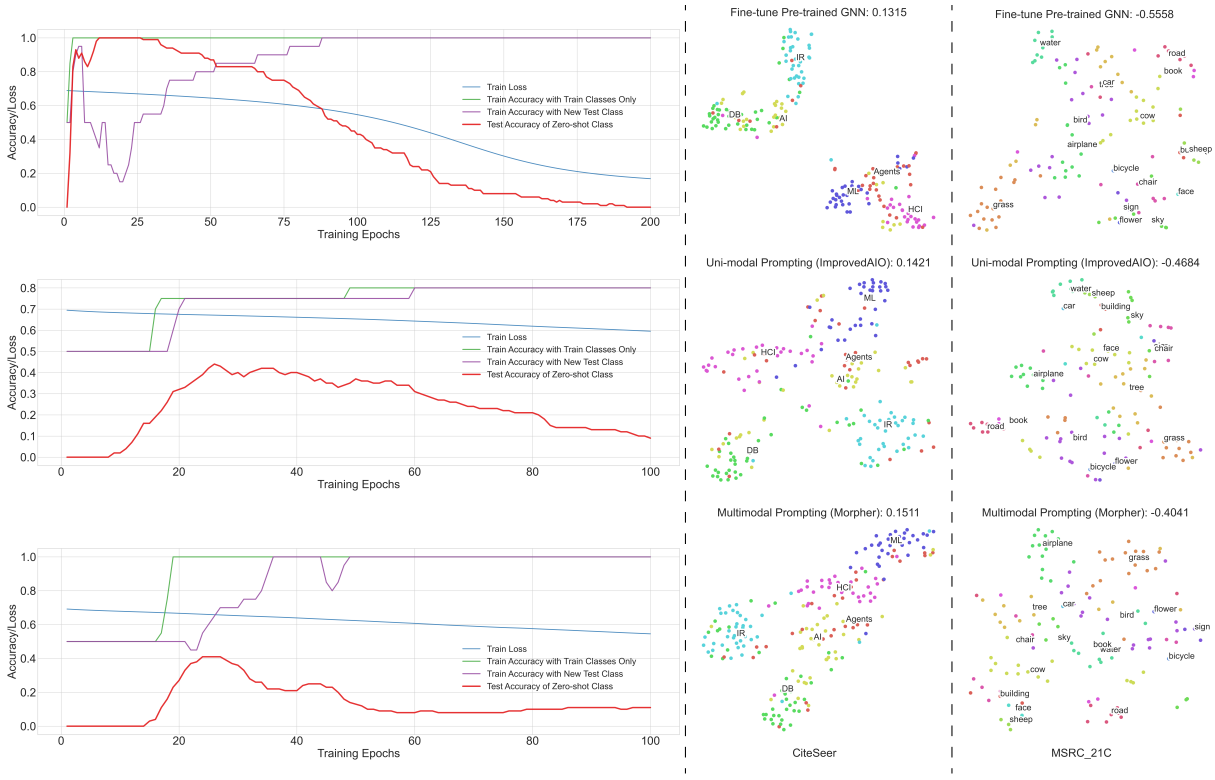

Figure 3: Results of novel class generalization (left); t-SNE embedding plots on CiteSeer, MSRC_21C (right). Train accuracy with train classes only is the accuracy of predicting the training graphs from the two training classes. Train accuracy with new test classes is the accuracy of predicting the training graphs from all three classes. Test Accuracy of zero-shot class is the accuracy of predicting the testing graphs from all three classes. Full-resolution figures can be found in Appendix D.

Target Domain		MUTAG		PubMed	
Target Task		graph-level		node-level	
Source	Methods	Acc	F1	Acc	F1
ENZYMES (graph-level)	Fine-tune	68.00	55.04	47.57	36.07
	ImprovedAIO	70.67	64.07	50.28	50.51
	Morpher	**72.67**	**73.29**	**54.42**	**53.96**
CiteSeer (node-level)	Fine-tune	71.33	62.19	48.71	40.66
	ImprovedAIO	74.00	73.76	52.57	51.29
	Morpher	**76.67**	**77.04**	**58.29**	**57.54**

Table 3: Domain Transfer Performance. Best results are bolded and second-best results are underlined.

5.4 Zero-shot Classification Prototype

An advantage of adapting pre-trained GNNs to the semantic embedding space is that GNNs might be empowered to "reasoning" in a CLIP style. Here, we conduct a novel experiment that generalizes GNN to an unseen class. Since no real-world data is available for this setting, we synthetically create three datasets, ZERO-Cora, ZERO-CiteSeer, and ZERO-PubMed, all from real-world connections. We aim to simulate a citation network with two research areas and an interdisciplinary research area in between. For each citation network, we randomly sample 120 nodes and induce their 2-hop ego-graphs and then replace the node features in 10 ego-graphs with $[1, 0]$ and another 10 ego-graphs with $[0, 1]$ to construct 20 training graph samples. For the remaining ego-graphs, we uniformly randomly replace the node features with $[1, 0]$ and $[0, 1]$ to construct 100 testing graph samples. We assign text labels of the first research area (e.g., "biology") to the $[1, 0]$ training graphs, the second research area (e.g., "informatics") to the $[0, 1]$ training graphs, and the interdisciplinary area (e.g., "bioinformatics") to the testing graphs. Intuitively, the nodes with feature $[1, 0]$ are papers in the first area, and nodes with feature $[0, 1]$ are in the second area, which makes the datasets rational.

For each dataset, using GraphCL+GCN, we pre-train GNNs on all graphs. Then, we train Morpher on the training graphs, only knowing the text labels of the two training classes. Since we do not have validation data in zero-shot learning, we report the results of each epoch in Figure 3 (left). We observe that, while Morpher quickly adapts the GNN to downstream training data, the CLIP-like framework can predict the graphs in the novel class

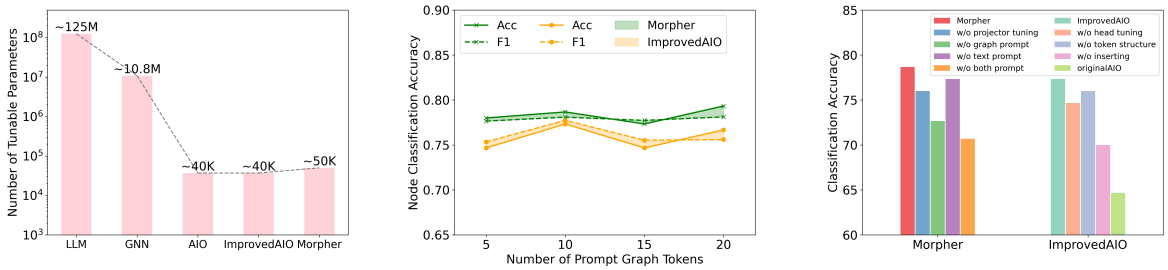

Figure 4: Efficiency comparison (left), parameter study (middle) and ablation study (right).

with good accuracy (red curve). Moreover, the training samples can be classified correctly from training and novel classes. Before the training overfits, there is a period when Morpher can distinguish all the graphs from the training and novel classes with high accuracy. Such zero-shot novel-class generalization ability validates Morpher's alignment between graph embeddings and text embeddings. When Morpher is trained on two classes of graphs with text labels of biology and informatics, a graph-in-the-middle will be classified as text-in-the-middle: bioinformatics, even if "bioinformatics" is an unseen label.

5.5 Efficiency and Embedding Analysis

Without fine-tuning the GNN or LLM, the prompt-based methods have better parameter efficiency. As shown in Figure 4 (left), our ImprovedAIO and Morpher require similar numbers of parameters with AIO (Sun et al., 2023a), which is 0.032% to 0.46% compared to either tune the LLM (RoBERTa) or GNN (GCN). Due to such parameter efficiency, our methods learn better graph representations given few-shot data. We visualize the graph embeddings of CiteSeer and MSRC_21C in Figure 3 and calculate the silhouette score, a metric for cluster quality ($\uparrow$) ranged in $[-1, 1]$. It turns out that our Morpher leads to better adaptation.

5.6 Hyperparameter and Ablation Study

We conduct the hyperparameter study by choosing and testing various numbers of graph prompt tokens for both ImprovedAIO and Morpher. The results are shown in Figure 4 (middle), from which we can observe that both methods are generally stable, and Morpher constantly outperforms ImprovedAIO under different choices. To verify the necessity of each component in our design, we compare Morpher and ImprovedAIO with multiple variants, respectively, and report the result in Figure 4 (right). We observe that removing any component would result in a performance drop.

We also conduct experiments to verify the effectiveness of our proposed Morpher with ELECTRA (Clark et al., 2020) and DistilBERT (Sanh et al., 2019) as the text encoder in Appendix B.3 due to space limitation. In general, Morpher is robust with respect to the language encoder. As for the robustness with respect to the pre-trained GNNs, we further conduct experiments using GNNs pre-trained from GraphMAE (Hou et al., 2022) and MVGRL (Hassani and Ahmadi, 2020). Due to the space limitation, the results are in Appendix B.4.

6 Related Work

GNN Pre-training. Recently, a surge of graph pre-training strategies have emerged (Hu et al., 2020a; Lu et al., 2021; Jing et al., 2021; Zhou et al., 2022a). The main idea of pre-trained graph models is to capture general graph information across different tasks and transfer this knowledge to the target task using techniques such as contrastive predictive coding (Khosla et al., 2020; Xia et al., 2022), context prediction (Hu et al., 2020b), and mutual information maximization (Sun et al., 2020). Different from these approaches, this paper aims to adapt pre-trained GNNs by leveraging multi-modal prompt learning techniques.

Graph Prompt Learning. Recent studies exploring prompt learning for GNNs mark a thriving research area (Sun et al., 2023b; Wu et al., 2023b). It is a promising way to adapt GNNs to downstream tasks through token-level (Fang et al., 2023; Tan et al., 2023; Chen et al., 2023a; Sun et al., 2022; Zhu et al., 2023) or graph-level (Sun et al., 2023a; Huang et al., 2023; Ge et al., 2023) prompting. Among all the existing methods, All-in-one (AIO) (Sun et al., 2023a) is the only algorithm to learn tunable graph prompts for multi-level downstream tasks (Table 6). Based on our improved AIO, we present a pioneer study to explore learning prompts

in multiple modalities simultaneously while keeping the pre-trained models frozen.

LLM on Graphs. LLMs' potential for graph-related tasks (Jin et al., 2023a) has been explored recently. The first category employs LLMs as pre-trained feature extractors to enhance GNNs (Duan et al., 2023; Chien et al., 2021; Zhu et al., 2021). The second category focuses on integrating graph structures directly into LLM architectures (Yang et al., 2021; Zhang et al., 2022b; Jin et al., 2023d,c). Despite these advancements, none of them have explored the collaboration between LLMs and GNNs with extremely weak text supervision and under graph prompt learning.

7 Conclusion

We present Morpher, the first multimodal prompt learning paradigm leveraging LLMs to semantically adapt pre-trained GNNs to downstream tasks with extremely weak text supervision. Addressing limitations of existing graph prompting techniques, we demonstrate through extensive experiments that Morpher excels in few-shot, multi-level tasks, and domain transfer. Notably, Morpher enables generalization to novel testing classes.

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8 Limitations

Our Multimodal graph prompt learning paradigm assumes the "pre-train + prompt" framework to learn transferable graph representations, yet there could be other paths to achieve graph-related foundation models. Also, graph prompt learning only works on the graph neural network architecture, and might not work for other architectures that are proposed in the future. Another limitation of this work is the requirement of language encoder. While RoBERTa is one of the most advanced encoder-only language models and can be considered an LLM with over 0.1B parameters, more recent LLMs such as Llama or Mistral cannot be used in Morpher because they are decoder-only LLMs and do not explicitly have an encoder.

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A Dataset Details

A.1 Dataset Statistics

Table 4 summarizes the statistics of the public real-world datasets, which we used in the few-shot experiments. For our synthetic datasets in the zero-shot prototype, we summarize their statistics in Table 5. As discussed in Section 5.4, the connections of our synthetic datasets are real, and we only replace the node feature by $[1, 0]$ and $[0, 1]$. The code to download the public data and the code to create synthetic data are provided in the supplementary materials.

A.2 Text Labels

When created, real-world graph datasets are usually coupled with textual meanings, but a common practice is to convert the textual meanings into numbers to create labels, which weakens the supervision of the graph data. For each real-world dataset, we convert the numerical labels back to text labels and feed into Morpher Language encoder through "[learnable text prompt] + [text label]". The mapping from the numbers to text labels for each dataset are provided as follows:

MUTAG. MUTAG is a dataset of nitroaromatic compounds, aiming to predict their mutagenicity on Salmonella typhimurium. Therefore, the mapping from numerical labels to text labels is: {0: non-mutagenic on Salmonella typhimurium, 1: mutagenic on Salmonella typhimurium}.

ENZYMES. ENZYMES aims to predict which subcategory each enzyme belongs to. The subcategories are: 0: oxidoreductases, 1: transferases, 2: hydrolases, 3: lyases, 4: isomerases, 5: ligases.

PROTEINS. PROTEINS is a dataset comprising proteins classified as either enzymes or non-enzymes. Therefore, the mapping is: 0: 'enzyme', 1: 'non-enzyme'.

MSRC_21C. Each graph in MSRC is constructed according to an image. The graph label is the image label. MSRC_21C contains 20 classes in MSRC, and "C" here means "Challenging" as the graphs(images) that are easy to classify has been filtered. The mapping from the numerical labels to text labels is: {0: building, 1: grass, 2: tree, 3: cow, 4: sheep, 5: sky, 6: airplane, 7: water, 8: face, 9: car, 10: bicycle, 11: flower, 12: sign, 13: bird, 14: book, 15: chair, 16: road}.

Cora. Cora is a citation network of papers in seven research areas. Each paper is labeled according to its corresponding research area. The mapping from the numerical labels to text labels is: {0: case based, 1: genetic algorithms, 2: neural networks, 3: probabilistic methods, 4: reinforcement learning, 5: rule learning, 6: theory}.

CiteSeer. CiteSeer is a citation network of papers, each labeled according to one of six research areas. The mapping from the numerical labels to text labels is: {0: Agents, 1: AI, 2: DB, 3: IR, 4: ML, 5: HCI}. We note that using abbreviations of the research area is not an issue because these abbreviations frequently appear, and the LLM tends to tokenize each of them as one token.

PubMed. PubMed is a collection of scientific publications from the PubMed database related to diabetes, classified into one of three categories. The mapping from the numerical labels to text labels is: {0: Diabetes Mellitus Experimental, 1: Diabetes Mellitus Type 1, 2: Diabetes Mellitus Type 2}.

Edge-level tasks. Cora, CiteSeer and PubMed can also be used as link prediction datasets. For link prediction, the mapping from the numerical labels to text labels is: {0: not connected, 1: connected}.

Synthetic Zero-shot Class Generalization Datasets. For ZERO-Cora, we synthetic three classes of ego-graph in a citation network. The first and second classes, respectively, have text labels "machine learning" and "theory", and the third (novel) class to generalize is "machine learning theory". For ZERO-CiteSeer, we synthetic three classes of ego-graph in a citation network. The first and second classes, respectively, have text labels "biology" and "informatics", and the third (novel) class to generalize is "bioinformatics". For ZERO-PubMed, we synthetic three classes of ego-graph in a citation network in the medical domain. The first and second classes, respectively, have text labels "cardiology" and "neurology", and the third (novel) class to generalize is "neurocardiology".

B Experiment Details

B.1 Reproducibility

Code. The code for the experiments is provided in the supplementary material with a well-written README file. We also provide the commands and instructions to run the code. The datasets used

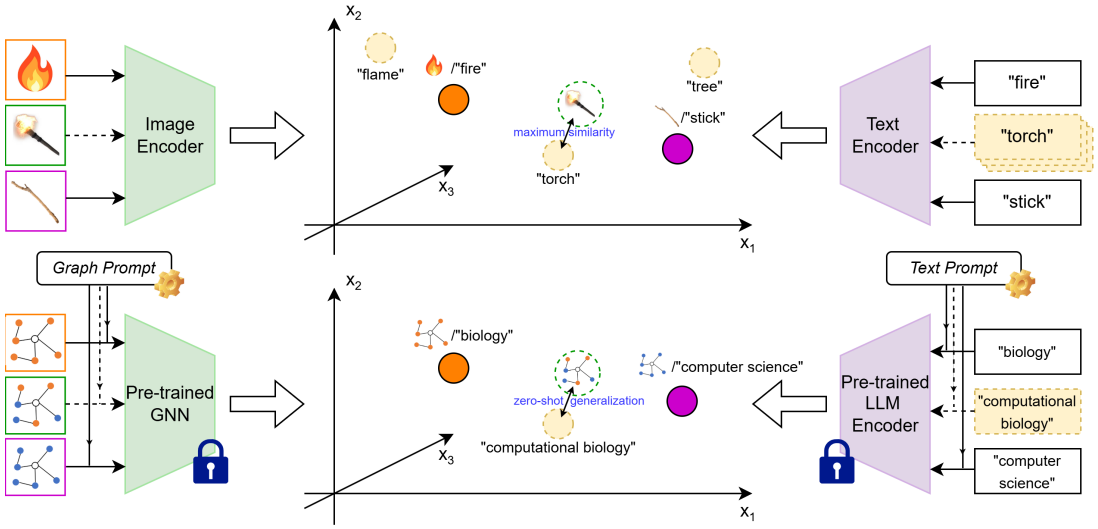


Figure 5: CLIP backbone (top) and this work (bottom). If a research paper cites many papers from biology and computer science, we realize this paper will likely be about computational biology, even if we do not know what exactly computational biology is. CLIP builds image encoders that learn such language dependency by Contrastive Language-Image Pre-training in the same embedding space according to Internet-scale data. However, text supervision is often extremely weak for graphs. This work leverages Multi-modal Prompt Learning for Graph Neural Networks that can effectively teach GNNs language dependency given few training samples with weak text supervision.

Table 4: Dataset statistics

Dataset	task level	# graphs	average # nodes	average # edges	# feature dimension	# classes	# shots per class	feature characteristic
MUTAG	graph	188	17.9	39.6	7	2	10	one-hot, sparse
ENZYMES	graph	600	32.6	124.3	3	6	10	one-hot, sparse
PROTEINS	graph	1113	39.1	145.6	3	2	10	one-hot, sparse
MSRC_21C	graph	209	40.28	96.60	22	17	1	one-hot, sparse
Cora	node, edge	1	2708	10556	1433	7	2 (node), 20 (edge)	sum 1, sparse
CiteSeer	node, edge	1	3327	9104	3703	6	2 (node), 20 (edge)	sum 1, sparse
PubMed	node	1	19,717	88648	500	3	10	TF-IDF value, dense

will be automatically downloaded when the code is executed.

Environment. We run all our experiments on a Windows 11 machine with a 13th Gen Intel(R) Core(TM) i9-13900H CPU, 64GB RAM, and an NVIDIA RTX A4500 GPU. We have also tested the code on a Linux machine with NVIDIA TITAN RTX GPU. All the code of our algorithms is written in Python. The Python version in our environment is 3.9.18. In order to run our code, one has to install some other common libraries, including PyTorch, PyTorch Geometric, pandas, numpy, scipy, etc. Please refer to our README in the code directory for downloading instructions.

We have optimized our code and tested that the space cost of the CPU memory is less than 16 GB, and the space cost of the graphics card is less than 6 GB. The execution time to run an experiment is less than 20 minutes on our machine.

B.2 Implementation Details

We provide the configuration files for the experiments to reproduce the results. We initialize the graph prompt using kaiming_initialization, and we initialize the text prompts through real token embeddings. We have tested multiple initializations, and they would not affect the overall results. Specifically, we initialize the text prompt for each dataset as follows.

MUTAG: “a graph with property”; ENZYMES: “this enzyme is”; PROTEINS: “this protein is”; MSRC_21C: “an image of”; Cora: “a paper of”; CiteSeer: “a paper of”; PubMed: “a paper of”; Edge tasks: “central nodes are”.

In our few-shot setting, we split the labeled data into training samples and validation samples at approximately 1:1. For all the parameters, we used the Adam optimizer, whose learning rate and weight decay are provided in the configuration files.

Table 5: Synthetic Zero-shot Class Generalization Dataset statistics

Dataset	# graphs	average # nodes	average # edges	#feature dimension	# classes	# shots per class
ZERO-Cora	120	8.41	10.38	2	2	10
ZERO-CiteSeer	120	10.03	21.31	2	2	10
ZERO-PubMed	120	20.33	41.75	2	2	10

Table 6: Comparison of graph prompts.

Method	prompt level	level of supported downstream tasks			learnable prompt	semantic
		node-level	edge-level	graph-level		
GPF-Plus (Fang et al., 2023)	token-level	√	×	×	√	×
Gprompt (Liu et al., 2023d)	token-level	√	×	√	√	×
VNT (Tan et al., 2023)	token-level	×	×	√	√	×
ULTRA-DP (Chen et al., 2023a)	token-level	√	×	×	√	×
GPPT (Sun et al., 2022)	token-level	√	×	×	√	×
SGL-PT (Zhu et al., 2023)	token-level	√	×	×	√	×
SAP (Ge et al., 2023)	graph-level	√	×	√	√	×
PRODIGY (Huang et al., 2023)	graph-level	√	√	√	×	×
All-in-one (AIO) (Sun et al., 2023a)	graph-level	√	√	√	√	×
ImprovedAIO (ours)	graph-level	√	√	√	√	×
Morpher (ours)	graph-level	√	√	√	√	√

B.3 Experiment with ELECTRA and DistilBERT

On the LLM pre-training side, RoBERTa is one of the most advanced encoder-only LLMs until now, and we have demonstrated the effectiveness with RoBERTa serving on the LLM side in the Morpher paradigm. Additionally, we conducted experiments with ELECTRA (Clark et al., 2020) and DistilBERT (Sanh et al., 2019). Using these two LLMs, Morpher can also achieve comparable performances to RoBERTa. The results are shown in Table 8 and in Table 7.

In general, using ELECTRA and DistilBERT results in similar performance compared to using RoBERTa, showing the robustness of Morpher with respect to the language encoder.

B.4 Experiment with GNNs trained using GraphMAE and MVGRL

In the main pages, we used GraphCL and SimGRACE to show that Morpher achieves better performance given a pre-trained GNN. Additionally, to further verify the robustness of Morpher over the pre-train method, we conducted experiments on the pre-trained GNNs using GraphMAE (Hou et al., 2022) and MVGRL (Hassani and Ahmadi, 2020). We use GCN as the GNN backbone and RoBERTa as the LLM encoder, and the results are reported in Table 9 and Table 10.

Using GraphMAE or MVGRL to pre-train the GNN, the trend of performance is similar to that when using GraphCL or SimGRACE. Also, ImprovedAIO and Morpher's performance is similar to that of pre-trained GNNs from GraphCL or SimGRACE and can still significantly outperform the pre-train + fine-tune baseline, showing the robustness of Morpher with respect to the pre-training strategy.

B.5 Morpher on MolecureNet with More Text Supervision

The relatively abundant labeled graph-text pairs in medical and biological domains have significantly accelerated research into training large models specifically tailored for these areas (Qiu et al., 2023). For example, (Park et al., 2022) pretrains the multimodal medical model MedGTX for Electronic Health Records (EHR) using the open-source EHR dataset MIMIC-III. Similarly, ProGen (Madani et al., 2020) trains a 1.2B-parameter language model on approximately 280M protein sequences. HyenaDNA (Nguyen et al., 2023) pretrains a genomic foundation model on the human reference genome with context lengths of up to 1 million tokens. Furthermore, (Singhal et al., 2022) introduces the MultiMedQA benchmark and per-

Table 7: Few-shot graph classification performance (%) of Morpher with ELECTRA (Clark et al., 2020) as language encoder. Other experiment settings are identical to the main experiment.

GNN pretraining	MUTAG		ENZYMES		PROTEINS		MSRC_21C	
	Acc	F1	Acc	F1	Acc	F1	Acc	F1
GraphCL + GCN	78.00	78.17	20.41	15.79	67.38	65.66	43.42	47.19
GraphCL + GAT	76.67	75.75	20.41	11.37	66.26	65.66	44.57	49.01
GraphCL + GT	76.67	77.04	19.16	14.68	73.06	72.70	42.28	44.09
SimGRACE + GCN	70.00	70.99	19.79	12.41	68.96	67.77	45.71	48.44
SimGRACE + GAT	77.33	77.51	18.12	13.31	68.96	67.78	44.00	49.43
SimGRACE + GT	72.67	73.55	18.33	15.76	70.18	70.28	41.14	44.50

Table 8: Few-shot graph classification performance (%) of Morpher with DistilBERT (Sanh et al., 2019) as language encoder. Other experiment settings are identical to the main experiment.

GNN pretraining	MUTAG		ENZYMES		PROTEINS		MSRC_21C	
	Acc	F1	Acc	F1	Acc	F1	Acc	F1
GraphCL + GCN	78.00	78.61	20.62	10.00	66.44	65.54	43.42	47.98
GraphCL + GAT	77.33	75.64	21.25	15.87	70.59	68.25	45.14	48.82
GraphCL + GT	74.67	75.20	19.58	14.96	70.27	70.55	44.57	47.28
SimGRACE + GCN	69.33	70.36	20.62	18.82	66.91	66.41	45.14	47.77
SimGRACE + GAT	77.33	76.90	18.54	14.44	67.56	65.08	45.71	44.36
SimGRACE + GT	72.67	73.52	17.91	11.06	70.55	70.36	45.14	44.01

forms instruction-tuning on the 540-billion parameter Flan-PaLM model within the clinical domain.

We demonstrate that, though not specifically designed for any downstream applications, the Morpher framework has the potential to be used in various tasks where there is more text supervision compared to previous experiments. As for a case study, We use bace (inhibitors of human beta-secretase), tox21 (toxicology in the 21st century) and hiv (inhibit HIV replication) from MolecureNet (Wu et al., 2017). These three datasets have 1513, 7831, and 41127 graphs to classify, respectively. In these datasets, each graph label is associated with a text description. The tasks on bace and hiv are bioactivity prediction and the task on tox21 is toxicity prediction. To adopt Morpher, we use GraphCL to pre-train the GAT model and initialize the text prompts and text labels using those from GIMLET (Zhao et al., 2023).

KVPLM (Zeng et al., 2022), MoMu (Su et al., 2022), Galactica-1.3B (Taylor et al., 2022) are zero-shot predictors for the three tasks; GIMLET-64M-50-shots is the GIMLET (Zhao et al., 2023) model fine-tuned on 50 additional training samples[2]; GAT-1M-fully-supervised uses all the training data to train a GAT. Our Morpher-k-shots uses only k training samples. From the results, first, using only 10 training samples, Morpher can outperform the zero-shot baselines KVPLM, MoMu, and Galactica-1.3B. Second, using only 50 shots, Morpher can achieve similar performance with the fully supervised GAT. Third, using the same amount of few-shot data (50 shots), Morpher-50 outperforms GIMLET-64M-50-shots on tox21 and hiv, the two largest datasets among the three. This means our graph-text multi-modal prompt learning, with much fewer learnable parameters ($\sim 50K$), is more sample-efficient than fine-tuning language model encoder.

[2]the performance of GIMLET and other baselines are directly from the GIMLET paper (Zhao et al., 2023).

B.6 Full Table for Few-shot Experiment

Due to the page limitation of the main pages, Table 14 shows the full table for the few-shot experiment.

B.7 Full Table for Domain Transfer

In the main pages, through the experiments presented in Tables 1 and 2, we have already demonstrated that fine-tune outperforms supervised, and ImprovedAIO significantly outperforms the original AIO. Therefore, in Table 3, we focus on comparing Morpher, ImprovedAIO and fine-tune methods to avoid redundancy. Here, we report the full comparison with the performance of supervised and AIO baselines. in Table 13. The result is consistent that fine-tune outperforms supervised, and our improvedAIO outperforms AIO.

We would like to acknowledge that AIO demonstrates state-of-the-art performance under the ex-

Table 9: Few-shot graph classification performance (%) of Morpher with the GNN pre-trained by GraphMAE (Hou et al., 2022). Other experiment settings are identical to the main experiment.

GNN pretraining	MUTAG		ENZYMES		PROTEINS		MSRC_21C	
	Acc	F1	Acc	F1	Acc	F1	Acc	F1
Pre-train + Fine-tune	71.33	71.41	16.04	12.14	65.86	65.22	39.42	40.20
ImprovedAIO	76.67	76.95	19.58	12.59	66.36	65.30	42.28	46.81
Morpher	78.67	78.67	20.20	16.95	67.38	65.66	45.71	48.49

Table 10: Few-shot graph classification performance (%) of Morpher with the GNN pre-trained by MVGRL (Hassani and Ahmadi, 2020). Other experiment settings are identical to the main experiment.

GNN pretraining	MUTAG		ENZYMES		PROTEINS		MSRC_21C	
	Acc	F1	Acc	F1	Acc	F1	Acc	F1
Pre-train + Fine-tune	68.67	69.46	16.45	10.16	65.15	64.71	38.85	40.56
ImprovedAIO	74.67	74.00	18.13	15.57	66.54	65.90	42.85	46.66
Morpher	78.00	77.81	18.96	14.97	67.56	66.79	44.57	48.67

perimental settings reported in its original paper (Sun et al., 2023a). However, our evaluation is conducted under more challenging conditions, particularly with fewer training and validation samples. In these settings, we observe that AIO's performance degrades, suggesting there is still room for improvement. To address this, we propose ImprovedAIO, which extends AIO's design to better handle these harder scenarios. Our goal is not to critique prior work, but to help advance the field of graph prompt learning and multimodal alignment by pushing toward more robust and generalizable solutions.

C Further Discussions

C.1 Unstable Training of Current Graph Prompt Design

As analyzed in Section 3, the current graph prompt design suffers from unstable training due to the imbalance of inner-connections and cross-connections because for any node i and token p_j, the dot products $\mathbf{X}(i,:)\mathbf{P}_\theta^g(j,:)^\top$ is close to 0, leading to ineffective prompt-token interactions. A potential solution to ensure $\mathbf{X}(i,:)\mathbf{P}_\theta^g(j,:)^\top$ has a larger nonzero value is to initialize prompt tokens with higher variance. Through further analysis and experimental validation, We tend to believe that it fails to address the root cause.

First, initializing parameters with high variance can introduce additional challenges during training, such as unstable gradients, over-reliance on the initial high-variance parameters, and ineffective weight regularization. Specifically, in the prompt learning setting, high-variance initialization of prompts may cause the training process to overly focus on the prompt embeddings, thereby overshadowing the information encoded in the input graph and hindering the model's ability to learn meaningful representations from the input graph structure.

Second, even with high-variance initialization, the computation of $\sigma(\mathbf{X}(i,:)\mathbf{P}_\theta^g(j,:)^\top)$ would still result in approximately half of the cross-connections being established. While this is an improvement over the original AIO, where nearly all cross-connections are formed, it would still lead to the prompted graph representations being overly similar. As a result, the task head cannot effectively learn to distinguish between different graphs.

To further validate this analysis, we conducted additional experiments using high-variance initialization in the original AIO method. These experiments were performed in the few-shot learning setting (Table 12) using GraphCL pretraining and a GAT encoder.

As shown in Table 12, increasing the initialization variance does not consistently improve performance. In some cases, it even leads to degradation, likely due to training instability. Furthermore, the overall performance of AIO remains significantly lower than that of our ImprovedAIO and Morpher, demonstrating that high-variance initialization is not a sufficient solution to the dense cross-connection issue.

Our ImprovedAIO effectively addresses the training issue of graph prompt learning without

Table 11: AUC-ROC (↑) on MolecureNet (bace, tox21, hiv). Morpher-K denotes K shots.

Dataset	KVPLM	MoMu	Galactica-1.3B	GIMLET-64M-50-shots	GAT-1M-supervised	Morpher-10	Morpher-20	Morpher-50
bace	0.5126	0.6656	0.5648	0.729	0.697	0.6231	0.6513	0.6858
tox21	0.4917	0.5757	0.4946	0.652	0.754	0.6769	0.7275	0.7459
hiv	0.6120	0.5026	0.3385	0.721	0.729	0.5742	0.7034	0.7283

	MUTAG	ENZYMES	PROTEINS	MSRC_21C
default variance	64.67	17.50	59.21	14.37
3× variance	64.67	17.50	61.79	13.17
5× variance	68.00	17.70	59.21	11.37
10× variance	67.33	16.45	58.65	17.96

Table 12: Accuracy results of high-variance initialization experiments in few-shot learning.

Target Domain		MUTAG		PubMed	
Target Task		graph-level		node-level	
Source	Methods	Acc	F1	Acc	F1
ENZYMES (graph-level)	Supervised	66.00	56.67	47.57	36.07
	Fine-tune	68.00	55.04	47.57	36.07
	AIO	64.00	54.50	44.85	34.13
	ImprovedAIO	<u>70.67</u>	<u>64.07</u>	<u>50.28</u>	<u>50.51</u>
	Morpher	**72.67**	**73.29**	**54.42**	**53.96**
CiteSeer (node-level)	Supervised	66.00	56.67	47.57	36.07
	Fine-tune	71.33	62.19	48.71	40.66
	AIO	65.33	57.20	45.71	34.39
	ImprovedAIO	<u>74.00</u>	<u>73.76</u>	<u>52.57</u>	<u>51.29</u>
	Morpher	**76.67**	**77.04**	**58.29**	**57.54**

Table 13: Domain Transfer Performance. Best results are bolded and second-best results are underlined.

introducing any new thresholding hyperparameters. Due to our pruning mechanism, ImprovedAIO is less sensitive to the choice of δ_{cross}. Specifically, a smaller δ_{cross} can safely be used in our framework, as it allows more cross edges to be initially introduced without affecting the final set of cross edges after pruning.

C.2 Scalability of GNNs and LLMs

The scalability of our proposed method across different sizes of GNNs and LLMs is an important consideration. However, the primary focus of this work is to introduce multimodal prompt learning for GNNs and validate the effectiveness of our novel paradigm, Morpher.

Regarding GNN scalability, the scale of a GNN is highly dependent on the total available samples for self-supervised pretraining. In our experiments, we employed GNNs with up to 10M parameters, which is already relatively large for the datasets we used. Notably, many recent works achieving state-of-the-art performance on similar classification tasks use GNNs of comparable or smaller scale (Skenderi et al., 2023; Giusti et al., 2023; Kreuzer et al., 2021; Frasca et al., 2022; Bouritsas et al., 2023).

For LLM scalability, as mentioned in the limitation section of our paper, our method requires a language encoder and has not yet been integrated with very large decoder-only LLMs. Nonetheless, our experiments with RoBERTa (0.1B parameters), ELECTRA (0.3B parameters), and DistilBERT (0.06B parameters) in our ablation study demonstrate that Morpher is robust across a variety of language encoders with different designs and scales.

Our contributions in this paper include improving the design of graph prompts and introducing a multimodal prompt learning paradigm for GNNs, tailored to real-world scenarios where text supervision is extremely weak. Through extensive experiments, we have demonstrated that our proposed methods outperform state-of-the-art baselines, establishing a robust and effective framework for multimodal learning. While scalability across larger GNNs and LLMs is an important direction, it is beyond the scope of this work and we highlight scalability as a potential future research to extend Morpher to even larger models.

C.3 Model and Data Scaling Laws

Scaling laws and emergence ability have attracted much research interest recently (Kaplan et al., 2020). To this end, we conduct additional experiments regarding the data scaling capability and model scaling capability using GraphCL+GCN on the MUTAG dataset.

Scaling law with respect to model size. Since our Morpher does not require the pretraining of large language models (LLMs), we report the performance using various LLMs of different sizes in Table 15. Next, we pre-train GNNs of varying sizes by adjusting parameters such as the hidden dimension, while keeping the language model fixed to RoBERTa, and report the results in Figure 16. Based on these results, we did not observe significant scaling laws with respect to the size of the LLM or GNN. We hypothesize that this may be because the sizes of the LLM and GNN have not yet reached the threshold for exhibiting emergent capa-

Training schemes	GNN pretraining	MUTAG		ENZYMES		PROTEINS		MSRC_21C	
		Acc	F1	Acc	F1	Acc	F1	Acc	F1
Supervised	N/A + GCN	66.00	66.67	16.67	8.68	65.89	60.77	38.85	35.32
	N/A + GAT	66.00	65.69	16.45	4.65	64.75	64.08	41.14	39.86
	N/A + GT	66.66	66.26	15.62	4.22	62.81	57.12	38.28	41.62
Pre-train + Fine-tune	GraphCL+GCN	70.00	70.23	17.91	11.82	65.89	61.23	40.00	43.89
	GraphCL+GAT	70.00	69.73	17.91	10.46	65.16	63.92	44.57	45.74
	GraphCL+GT	68.00	67.81	17.70	8.99	63.28	56.41	41.71	43.73
	SimGRACE+GCN	66.67	67.27	17.29	8.78	66.82	64.70	40.57	43.84
	SimGRACE+GAT	70.67	69.10	16.87	7.18	65.42	63.65	42.85	42.37
	SimGRACE+GT	69.33	69.77	16.24	6.08	65.98	62.31	39.42	40.78
AIO (Sun et al., 2023a)	GraphCL+GCN	64.67	39.27	17.50	4.97	61.35	44.93	3.59	10.09
	GraphCL+GAT	64.67	39.27	17.50	4.97	59.21	37.19	14.37	3.11
	GraphCL+GT	73.33	72.06	18.33	9.09	40.79	28.97	17.96	8.30
	SimGRACE+GCN	64.67	39.27	16.04	4.61	67.42	60.87	34.73	18.16
	SimGRACE+GAT	64.67	39.27	16.04	4.61	59.21	37.19	7.78	1.79
	SimGRACE+GT	36.00	27.26	17.50	8.15	50.56	49.34	32.34	15.13
GPF-plus (Fang et al., 2023)	GraphCL+GCN	68.67	67.27	16.88	15.48	64.75	61.45	47.42	29.02
	GraphCL+GAT	68.67	62.84	16.45	13.23	65.89	60.07	47.42	26.28
	GraphCL+GT	69.33	67.87	18.12	15.56	59.66	37.37	41.71	21.35
	SimGRACE+GCN	65.33	39.52	18.96	15.83	65.16	58.80	45.71	23.32
	SimGRACE+GAT	69.33	66.72	18.54	12.58	63.28	53.50	42.85	21.40
	SimGRACE+GT	70.00	67.31	17.91	14.69	64.83	52.97	34.13	20.13
Gprompt (Liu et al., 2023d)	GraphCL+GCN	73.33	66.93	17.91	8.44	61.01	60.01	1.80	0.21
	GraphCL+GAT	64.67	62.63	17.08	14.18	50.56	50.55	1.80	0.22
	GraphCL+GT	70.67	70.02	17.91	9.64	63.28	58.65	1.80	0.21
	SimGRACE+GCN	65.33	39.52	17.29	14.48	52.70	52.68	1.80	0.21
	SimGRACE+GAT	67.33	65.88	16.25	11.31	59.10	58.72	1.80	0.21
	SimGRACE+GT	73.33	67.84	16.87	13.54	64.75	62.37	1.80	0.223
Improved AIO (Ours)	GraphCL+GCN	77.33	77.74	18.13	11.98	65.89	65.97	42.85	45.91
	GraphCL+GAT	74.67	75.51	18.33	11.26	65.76	66.05	46.85	51.39
	GraphCL+GT	74.67	74.67	19.16	9.04	68.12	68.18	42.85	43.54
	SimGRACE+GCN	68.00	69.01	17.91	9.02	66.82	66.40	44.57	49.24
	SimGRACE+GAT	77.33	77.20	18.75	9.39	66.91	65.49	45.14	42.31
	SimGRACE+GT	71.33	72.06	18.95	11.25	68.59	68.84	40.57	42.82
Morpher (Ours)	GraphCL+GCN	78.67	78.09	20.41	15.20	67.47	66.40	45.14	49.62
	GraphCL+GAT	79.33	79.15	23.12	18.01	70.89	70.30	50.85	54.48
	GraphCL+GT	76.00	76.51	19.58	13.28	73.53	72.48	45.71	48.41
	SimGRACE+GCN	69.33	70.27	19.79	14.94	67.10	66.15	45.71	51.24
	SimGRACE+GAT	78.00	77.65	20.21	16.27	68.12	67.26	45.71	51.13
	SimGRACE+GT	74.00	74.84	19.16	14.29	71.76	71.75	44.00	48.16
IMP of ImprovedAIO		2.00 ↑	5.01 ↑	0.52 ↑	4.41 ↓	2.01 ↑	4.37 ↑	0.28 ↓	2.50 ↑
IMP of Morpher		4.00 ↑	6.73 ↑	2.36 ↑	0.60 ↑	4.81 ↑	6.61 ↑	2.66 ↑	7.14 ↑

Table 14: Few-shot graph classification performance (%). IMP (%): the average improvement (absolute value) compared to the **best result** among all the baseline methods.

bilities. Further investigation into this phenomenon is an interesting direction for future work.

Language Model Size	MUTAG Acc	MUTAG F1
DistilBERT 0.06B	78.00	78.61
RoBERTa 0.1B	78.67	78.09
ELECTRA 0.3B	78,00	78.17

Table 15: Scaling law with respect to language model size.

GCN Model Size	MUTAG Acc	MUTAG F1
1M	78.00	78.56
3M	78.67	78.97
10M	78.67	78.09

Table 16: Scaling law with respect to GCN model size.

Scaling law with respect to data size We conducted additional studies by adjusting either the pre-training data size or the downstream few-shot data size. To evaluate the effect of pre-training data size, we used GraphCL+GCN on the MUTAG dataset, randomly selecting k% of the samples for GNN pre-training. The results are presented in Table 17. The results suggest that increasing the size of either the pre-training data or the downstream few-shot data generally improves the performance of our Morpher. This observation is consistent with typical data scaling laws. While the current findings provide valuable insights, further investigation is required to explore the detailed effects of data scaling, which we leave for future work.

Pretrain Data Ratio	MUTAG Acc	MUTAG F1
10%	72.00	68.80
30%	75.33	75.11
100%	78.67	78.09

Table 17: Scaling law with respect to data size.

C.4 Tunable pre-trained GNN/LLM Scenario

Generally, in NLP, prompt or prefix tuning is often employed as a parameter-efficient alternative to fine-tuning, especially when fine-tuning the entire model is computationally expensive. While prompt tuning and fine-tuning are not technically incompatible, they are typically not used simultaneously, as the goal of prompt tuning is to achieve strong performance without the need to update the entire model.

That being said, making the pre-trained GNN tunable could potentially further enhance performance in specific scenarios. However, this would come at the cost of increased computational complexity and resource requirements, which goes against the motivation of our proposed method. We designed Morpher with efficiency in mind, ensuring that it achieves strong performance without requiring extensive updates to the pre-trained GNN. Furthermore, given the weak text supervision in our setting, increasing the parameter space by making the GNN tunable could reduce the sample efficiency of prompt tuning, potentially hindering the model's ability to learn effectively from limited supervision.

Therefore, while the scenario where the GNN—and potentially the language model—are also tunable is an interesting direction, it falls beyond the scope of this paper. Nonetheless, we acknowledge this as an open question that warrants further exploration in future research, particularly to better understand the trade-offs between parameter efficiency and model expressiveness.

C.5 Broader Impact and Future Directions

Learning on graphs has been a long-standing goal in the machine learning community, evolving from pattern-based mining (Li et al., 2025a) to modern graph neural network models (Zheng et al., 2024b; Wang et al., 2025), with broad applications in social network analysis (Li et al., 2023b; He et al., 2024), natural sciences (Fu et al., 2025), and beyond (Li et al., 2024a; Fu et al., 2024a; Li et al., 2024b; Lin et al., 2025a; Jin et al., 2024). In addition to advancing graph-language alignment and graph prompt learning, we hope this work can also inspire future research in the following directions.

Distribution Shift in Graph Data. Real-world graph data often undergoes distribution shifts in both node features and graph structures, which can severely degrade the performance of GNNs. Before foundational GNNs, to address this challenge, graph domain adaptation aims to adapt a pretrained GNN model to a target graph via either model adaptation (Bao et al.; Wu et al., 2023a; Guo et al., 2022; Tieu et al., 2025) or data adaptation (Liu et al., 2023b; Wei et al., 2022; Lin et al., 2024; Zeng et al., 2025; He et al., 2025b).

Graph Foundation Models versus Domain Specific GNNs. In the era of big data and AI (Liu et al., 2020; Wei et al., 2020; Liu et al., 2025; Fu et al., 2024b; Zou et al., 2025; Zhang et al., 2025),

graph foundation models play an important role in many applications, such as network alignment (Yan et al., 2021, 2022; Zeng et al., 2024; Yu et al., 2025), spectral graph signal processing (Xu et al.; Liu et al., 2024b), anomaly detection (Zheng et al., 2025, 2024a), multi-layered network embedding (Yan et al., 2024a,b,c; Jing et al., 2022, 2024), information retrieval (Wei et al., 2021; Yoo et al., 2024; Liu et al., 2024a) and time series analysis (Roach et al., 2020; Fu et al., 2022; Wang et al., 2023; Lin et al., 2025b; Ban et al., 2024; Tieu et al., 2024; Fu et al., 2024c). However, as noted earlier, graph foundation models still face challenges under distribution shifts. In practice, many real-world applications continue to rely on domain-specific GNN solutions when sufficient training data is available. While this work introduces a method for training graph foundation models under extremely weak text supervision, we still recommend evaluating domain-specific GNNs as a baseline when developing real-world systems.

Multimodal Learning with Graphs. Multimodality learning (Zheng et al., 2021, 2023; Li et al., 2025b; Wei et al., 2024) has been studied for decades. Inspired by the success of large language model (Radford et al., 2021; Lan et al., 2024; Ai et al., 2025), a new trend of multimodal learning with graphs (Zheng et al., 2024c; He et al., 2025a) is to align the text representation with graph structure for text-attributed graphs (Wen and Fang, 2023) or bridge molecular graphs and text data with semantic alignment for text-paired graphs (Liu et al., 2023e). Our work presents an alignment with graphs and languages, and similar frameworks can be expanded into graphs with other modalities.

Semantic-aware Graph Generative Modeling. Graph generation models (Kong et al., 2023; Vignac et al., 2022; Xu et al., 2024; Zeng et al., 2023) have a longstanding history with wide applications in many domains. These methods aim to capture and reproduce one or more important structure properties, such as community structure (Zhou et al., 2019), motif distribution (Zheng et al., 2024e), and densification in graph evolution (Zhou et al., 2020). In this work, we present a prototype of a semantic-aware graph predictive model, and semantic-aware graph generative models could also be a future direction, which may hold great potential in conditioned generation.

D Full-Resolution Figures

Due to space constraints in the main text, we resized the figures for a more compact presentation in Figure 3. We provide the full-resolution versions of the figures here for finer details.

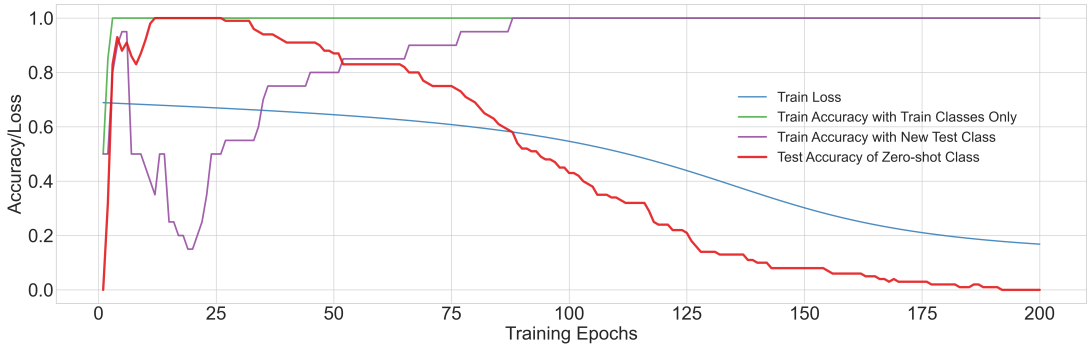


Figure 6: Novel class generalization result for our ZERO-Cora dataset.

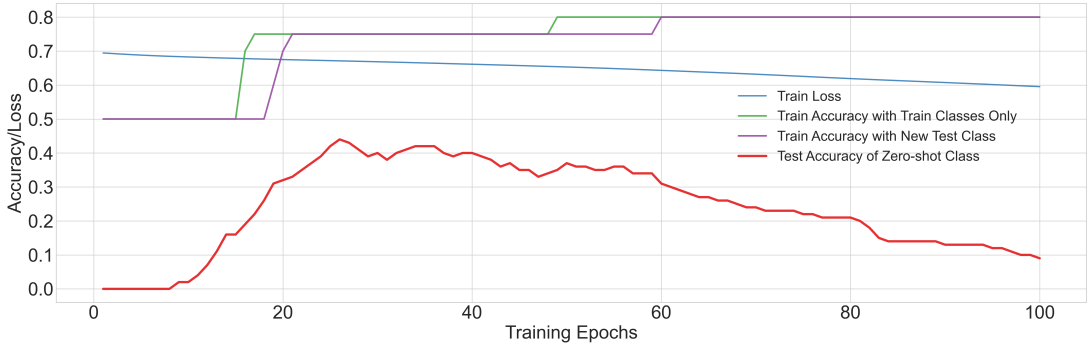


Figure 7: Novel class generalization result for our ZERO-CiteSeer dataset.

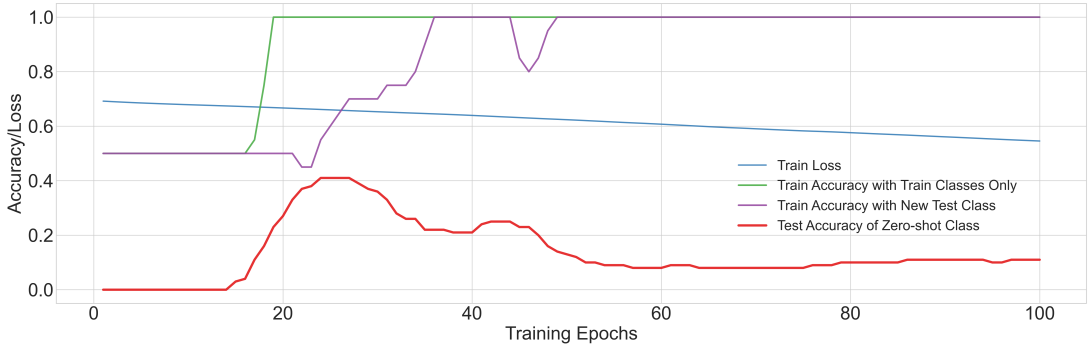
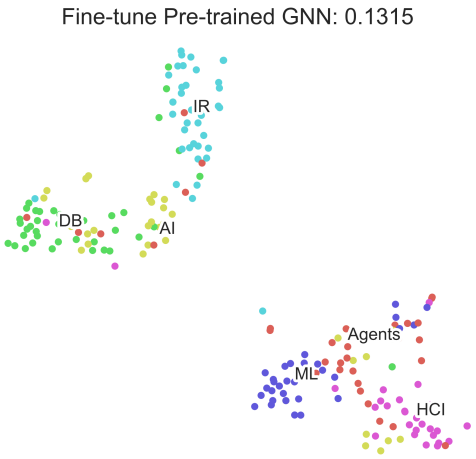
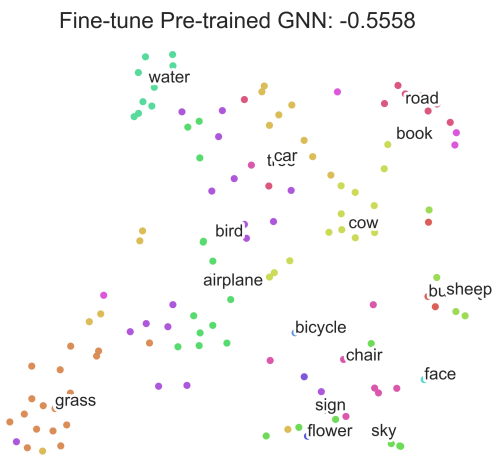


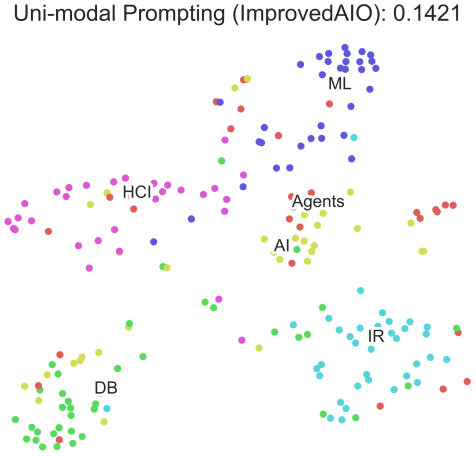
Figure 8: Novel class generalization result for our ZERO-PubMed dataset.



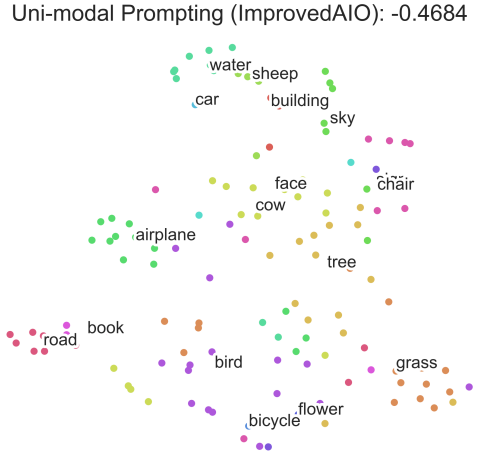
(a) Fine-tune on CiteSeer



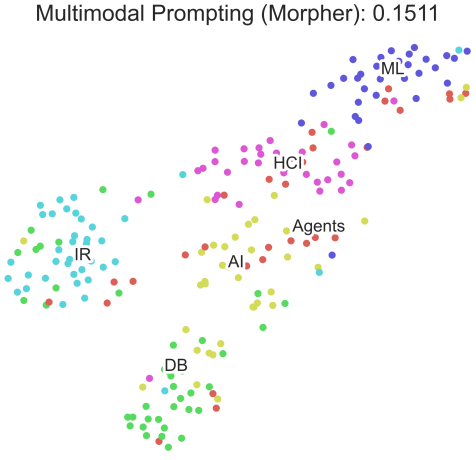
(b) Fine-tune on MSRC_21C



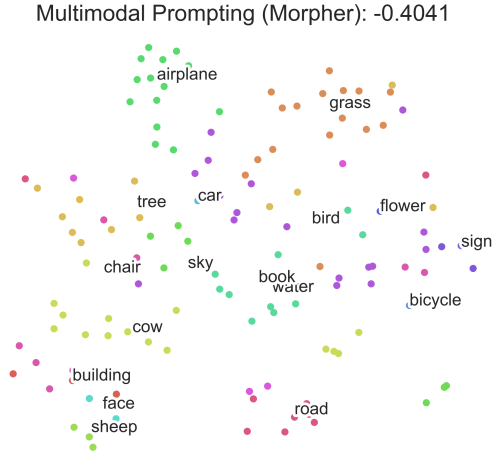
(c) ImprovedAIO on CiteSeer



(d) ImprovedAIO on MSRC_21C



(e) Morpher on CiteSeer



(f) Morpher on MSRC_21C

Figure 9: t-SNE embedding plots on CiteSeer (left) and MSRC_21C (right). We calculate the silhouette score, a metric for cluster quality (↑) ranged in $[-1, 1]$. It turns out that our Morpher leads to better adaptation.