# Towards Graph Prompt Learning: A Survey and Beyond

Qingqing Long\*, Yuchen Yan\*, Peiyan Zhang, Chen Fang, Wentao Cui, Zhiyuan Ning, Meng Xiao, Ning Cao, Xiao Luo, Lingjun Xu, Shiyue Jiang, Zheng Fang, Chong Chen, Xian-Sheng Hua and Yuanchun Zhou<sup>†</sup>

Abstract—Large-scale "pre-train and prompt learning" paradigms have demonstrated remarkable adaptability, enabling broad applications across diverse domains such as question answering, image recognition, and multimodal retrieval. This approach fully leverages the potential of large-scale pre-trained models, reducing downstream data requirements and computational costs while enhancing model applicability across various tasks. Graphs, as versatile data structures that capture relationships between entities, play pivotal roles in fields such as social network analysis, recommender systems, and biological graphs. Despite the success of pre-train and prompt learning paradigms in Natural Language Processing (NLP) and Computer Vision (CV), their application in graph domains remains nascent. In graph-structured data, not only do the node and edge features often have disparate distributions, but the topological structures also differ significantly. This diversity in graph data can lead to incompatible patterns or gaps between pre-training and fine-tuning on downstream graphs. We aim to bridge this gap by summarizing methods for alleviating these disparities. This includes exploring prompt design methodologies, comparing related techniques, assessing application scenarios and datasets, and identifying unresolved problems and challenges. This survey categorizes over 100 relevant works in this field, summarizing general design principles and the latest applications, including text-attributed graphs, molecules, proteins, and recommendation systems. Through this extensive review, we provide a foundational understanding of graph prompt learning, aiming to impact not only the graph mining community but also the broader Artificial General Intelligence (AGI) community. This survey underscores the potential of graph prompt learning for future research and practical applications, paving the way for advancements in this promising area.

Index Terms—graph prompt learning, graph pre-training, graph learning, graph fine-tuning, artificial general intelligence.

# 1 Introduction

In recent decades, the rapid advancement of artificial intelligence (AI) has facilitated its widespread application across various domains [1]–[3]. Graphs, as a distinctive data structure capable of describing general relationships between entities, have found extensive use in numerous real-world scenarios, including social network analysis [4]-[6], recommendation systems [7]-[10], and the chemical industry [11], [12]. To uncover the latent patterns within graph data and support downstream tasks, graph representation learning has emerged as a primary focus in the field of graph analysis [13], [14]. Given the non-Euclidean and high-dimensional nature of graph data, direct analysis of raw graphs poses significant challenges [15]–[17]. Graph representation learning addresses this issue by compressing graph data into low-dimensional Euclidean space, where vectors effectively represent the structure and properties of graphs [18], [19].

Traditional methods for graph representation learning primarily embed nodes into low-dimensional spaces based

 Qingqing Long, Chen Fang, Wentao Cui, Zhiyuan Ning, Meng Xiao, and Yuanchun Zhou: Computer Network Information Center, Chinese Academy of Sciences. University of Chinese Academy of Sciences. Email: {qqlong,fc,cuiwentao,ningzhiyuan,shadow,zyc}@cnic.cn

Yuchen Yan, Lingjun Xu, Shiyue Jiang, and Zheng Fang: Peking University. Email: {yyc,xlj,y1315508494,fang\_z}@stu.pku.edu.cn

 Peiyan Zhang, Ning Cao, Xiao Luo are from the University of Hong Kong, Nanyang Technological University, University of California Los Angeles, respectively. Chong Chen and Xian-Sheng Hua are from the Terminus Group. Email: pzhangao@cse.ust.hk, s210089@e.ntu.edu.sg, xiaoluo@cs.ucla.edu, chenchong.cz@gmail.com, huaxiansheng@gmail.com.

 \* represents the equally contributed authors, and † represents the corresponding author. on the graph adjacency matrix [20], [21]. With the evolution of deep learning, Graph Neural Networks (GNNs) have introduced novel solutions for graph representation learning [22], [23]. The core concept behind GNNs is message passing, which integrates local structural features into node attributes [13], [24]. Despite their success in various applications, GNNs predominantly rely on a supervised training paradigm, which depends on extensive labeled datasets to learn patterns between data samples and annotations for specific tasks [25]. However, data annotation is both time-consuming and often requires expert knowledge, posing challenges to scalability for large datasets [16]. Moreover, supervised learning approaches are susceptible to overfitting, which can adversely impact downstream performance [26].

Recently, self-supervised learning has achieved significant success in fields such as Natural Language Processing (NLP) [27], Computer Vision (CV) [28], and Recommender Systems (RecSys) [29]. Inspired by these advancements, there has been increasing interest in adapting the "pretraining and fine-tuning" paradigm to the graph domain [30], [31]. This approach leverages task-agnostic information to create pretext tasks for model initialization, followed by fine-tuning on target tasks with fewer labeled samples [26]. The knowledge gained from extensive pretext datasets enhances the model's generalization capabilities for specific target problems [32]. Within the "pre-train, fine-tune" framework, researchers focus on designing pretext task objectives and aligning them with target problems [33].

Graph prompt learning, an innovative extension of prompt engineering, applies the principles of prompt-based learning—widely studied in NLP—to the graph domain [27],

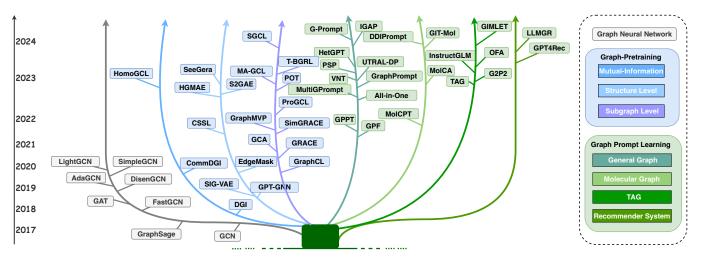


Fig. 1: Evolution of selected methods over the past eight years, where colored branches indicate different lines of methods.

[34]. Prompt engineering involves augmenting the input of large-scale pre-trained models with task-specific hints, i.e., prompts [28]. These prompts could be manually crafted natural language instructions, automatically generated instructions, or vector representations, which are referred to as discrete (hard) prompts and continuous (soft) prompts, respectively. This method has gained prominence due to its ability to adapt pre-trained models to new tasks with minimal labeled data and without extensive parameter tuning.

The primary advantage of graph prompt learning lies in its ability to efficiently leverage large pre-trained models for graph-related tasks. By providing task-specific prompts, these models can be guided to perform new tasks using their existing knowledge base. This approach significantly reduces the need for extensive labeled data and computational resources typically required for fine-tuning. Furthermore, it allows a single pre-trained model to be utilized for a wide range of downstream tasks, enhancing its applicability in real-world scenarios.

While prompt engineering has been extensively studied and applied in NLP and CV, its application in graph learning remains relatively unexplored. This survey aims to bridge this gap by providing a comprehensive overview of graph prompt learning. We classify the various prompting methods into categories based on their design and application, and we discuss the unique challenges and opportunities presented by this approach in the graph domain.

The remainder of this paper is organized as follows. In Section 4, we summarize the basic prompt design methodologies, including token design principles, task alignment mechanisms, and prompt tuning methods. Section 5 introduces general methods of homogeneous and heterogeneous graph prompting and summarizes their downstream applications, such as in molecular analysis, recommendation systems, and large language models (LLMs). Section 6 reviews benchmark datasets and evaluation methods, categorizing datasets into homophilous and heterophilous graphs and discussing specific evaluation criteria for tasks such as node classification, graph classification, and link prediction. We also highlight challenges related to dataset descriptions and the need for

standardized evaluation methods. In Section 7, we discuss the unresolved problems and future work, addressing the limitations of current graph prompt methods and proposing directions for deeper theoretical understandings. Through this survey, we aim to provide a foundational understanding of graph prompt learning, highlighting its potential for future research and applications. By addressing the current limitations and exploring new methodologies, we hope to advance the field and unlock new possibilities for graph representation learning.<sup>1</sup>

In comparison with existing surveys, this survey has three inclusive traits: (1) Novel Taxonomy: This work systematically examines the research works in the field of graph prompt learning and proposes a new classification. We first outline the design principles into three parts, i.e., prompting tokenization, alignment strategy between pretraining and downstream tasks, and prompt tunning strategy. We then discuss these principles in the context of both homogeneous and heterogeneous graphs. Finally, we summarize the applications of graph prompt learning, which include textattributed graphs, molecules, proteins, and recommendation systems. This is the first time such a classification has been proposed, providing a new perspective on the organization and categorization of graph prompt learning techniques. (2) Up-to-date Summarization: Graph prompt learning is a newly proposed concept, emerging around 2023. Thus, we have collected the most recent and relevant papers from 2023 to 2024, ensuring that our survey reflects the latest developments and state-of-the-art research in this rapidly evolving field. (3) Thorough Discussions: Based on the latest research, this survey offers a thorough discussion encompassing the background, design principles, benchmark datasets, and the latest applications of graph prompt learning. We showcase the latest and significant breakthroughs, analyze the current challenges, and provide insights to help readers grasp key concepts and principles, facilitating a deep understanding.

The **broader impact** of our work is twofold: (1) To <u>Graph Community</u>. Our survey serves as a valuable resource for machine learning researchers focusing on graph-

 $<sup>1. \ {\</sup>rm Figure} \ 1$  illustrates the evolution of selected methods over the past five years.

structured data. It can guide them in solving graph-related scientific problems, fostering innovation and knowledge discovery in this area. (2) To broader <u>AGI-related Community</u>. Our survey offers a detailed summary of important approaches in the field of "pre-train and prompt learning", providing valuable insights for researchers in AGI-related fields. By highlighting the design principle and practical applied implementations, our survey aids researchers in understanding and leveraging these techniques. This cross-disciplinary knowledge transfer can stimulate new ideas and solutions, ultimately contributing to advancements in AGI and its various applications.

#### 2 TAXONOMY

This section introduces the terms and notations related to Graph Prompt Learning that are used throughout the paper.

## 2.1 Terminology

In this section, we outline essential terms and their descriptions. Instead of providing formal definitions, we offer general explanations for clarity.

- *Graph Prompt*: A directive or cue included in the input of a pre-trained graph model to assist in executing specific tasks. These prompts can take the form of task-oriented instructions, handcrafted natural language directives, or vector-based representations.
- Prompting Method: A strategy used to embed prompts into the input, aiming to guide the model's actions and improve its performance.
- Prompt Tuning: The process of optimizing prompts to maximize the model's performance on specific tasks. This involves adjusting the prompts based on task requirements and model responses.
- Graph Neural Networks: A class of neural networks designed to work with graph-structured data. GNNs use message passing to integrate local structural features into node attributes.
- Self-Supervised Learning: A learning paradigm where the model learns to predict part of the data from other parts of the data. It does not require labeled data, which makes it suitable for large-scale, unlabeled datasets.
- Pre-Training and Fine-Tuning: A dual-phase training approach where a model is first pre-trained on an extensive, general-purpose dataset to acquire broad features. Subsequently, the model is fine-tuned on a more focused, task-specific dataset to tailor its capabilities to particular tasks.

## 2.2 Notations

We introduce the mathematical notations used throughout the paper in this section. All formulations in this work adhere to these notations unless otherwise specified. Consider an attributed graph  $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{X})$ , in which  $\mathcal{V} = v_1, v_2, \ldots, v_{|\mathcal{V}|}$  represents the set of nodes,  $\mathcal{E} \subset \mathcal{V} \times \mathcal{V}$  represents the set of edges, and  $\mathbf{X}$  denotes the feature matrix. Each node  $v_i$  in the graph has an associated attribute vector  $x_i \in \mathbb{R}^F$ , where F represents the dimension of the attribute vector. The collection of attribute vectors for all nodes forms the feature matrix  $\mathbf{X} \in \mathbb{R}^{|\mathcal{V}| \times F}$ . The edges can also be represented by an

adjacency matrix  $\mathbf{A} \in \mathbb{R}^{|\mathcal{V}| \times |\mathcal{V}|}$ , where  $\mathbf{A}_{ij} = 1$  if  $(v_i, v_j) \in \mathcal{E}$  and  $\mathbf{A}_{ij} = 0$  otherwise. Thus, the graph can alternatively be represented as  $\mathcal{G} = (\mathbf{A}, \mathbf{X})$ .

## 2.3 Literature Overview

This paper will be organized as follows:

In Section 3, we explore the foundational aspects of graph prompt learning. We begin by discussing the essential token designations within the graph domain, which encompass node token design, structure token design, and task token design. We then examine how these tokens are embedded into graph-related tasks, addressing both node-level alignment and graph-level alignment. Subsequently, we delve into advanced fine-tuning strategies for prompt learning, including pre-training models and integrating meta-learning techniques to enhance performance and adaptability.

Section 4 provides an extensive review of existing graph prompt learning methodologies, categorized into homogeneous and heterogeneous prompt learning. For homogeneous prompt learning, we investigate three critical dimensions: i) the integration of prompts as model inputs, ii) the enhancement of model outputs facilitated by prompts, and iii) the incorporation of supplementary information beyond mere attributes and structure into graph prompts. In the context of heterogeneous graph prompt methods, we focus on i) the design and application of prompts for heterogeneous tokens and message-passing processes, and ii) the impact of these prompts on improving the efficacy of heterogeneous graph tasks.

In Section 5, we delve into the diverse applications of graph prompt technology. We primarily address three prominent areas: i) the application of prompts in molecular graph analysis, where prompt learning aids in understanding complex molecular interactions; ii) the application of prompts in Text-Attributed Graphs, enhancing the integration and analysis of textual and structural data; and iii) the application of prompts in recommender systems, where prompts contribute to more personalized and accurate recommendation algorithms.

Section 6 is devoted to summarizing the common benchmarks, datasets, and experimental metrics used in the evaluation of graph prompt learning techniques. We provide a detailed comparison of various evaluation criteria tailored to different graph-related tasks, highlighting their strengths and limitations.

In Section 7, we address several challenging problems currently faced in the field of graph prompt learning. We also outline potential future research directions, emphasizing the need for innovative solutions and continued advancements to overcome existing limitations and to further enhance the applicability and robustness of graph prompt learning methodologies. Finally, we conclude our survey in Section 8.

#### 3 Connection to Related Techniques

This section presents a comparative analysis of graph prompt learning against relevant existing technologies to elucidate its distinctive features and advantages. We conduct two primary comparisons: (1) graph prompt learning versus graph pretraining/fine-tuning; (2) graph prompt learning in relation to

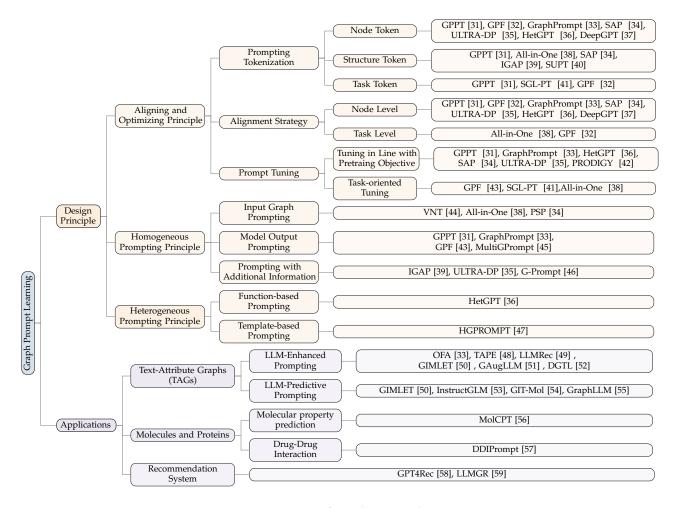


Fig. 2: A taxonomy of graph prompt learning.

graph few-shot learning. These comparisons aim to provide a comprehensive understanding of graph prompt learning's position within the current technological landscape.

# 3.1 Comparision with Graph Pre-training/Fine-tuning

Graph pre-training [35], [36] leverages large-scale graph datasets to learn generalizable representations, capturing intrinsic graph properties and topological patterns [37]. This unsupervised learning phase yields models with enhanced adaptability across diverse graph domains. The subsequent fine-tuning process optimizes these pre-trained models for specific tasks, exploiting the acquired structural knowledge to improve performance. This transfer learning approach enables efficient adaptation to novel graph problems, reducing the need for extensive task-specific data and training. The two-stage paradigm—pre-training followed by fine-tuning—significantly enhances the effectiveness of graph neural networks (GNNs) in various graph-based applications, from molecular modeling to social network analysis.

Taking the node classification task as an example, let  $g_{\theta}$  denote the pre-trained GNNs, and  $\mathcal{G}$  denote the graph of downstream tasks, i.e.,  $\mathcal{G} = \{\mathcal{V}, \mathcal{E}, \mathcal{X}, \mathcal{A}\}$  represent a graph with n nodes, where:  $\mathcal{V} = \{v_i\}_{i=1}^n$  is the node set,  $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$  defines the edge set,  $\mathcal{X} \in \mathbb{R}^{n \times d}$  denotes the d dimensional node feature matrix,  $\mathcal{A} \in \mathbb{R}^{n \times n}$  is the

adjacency matrix such that  $\mathcal{A}_{ij}=1$  if  $(v_j,v_j)\in\mathcal{E}$ , and 0 otherwise. And let [i] denote the node index of node  $v_i$ , and  $\mathcal{D}$  denote the label distribution of downstream tasks, i.e.,  $\mathcal{D}=\{(v_1,\mathcal{Y}_1),...,(v_n,\mathcal{Y}_n)\}$ . Then the pre-training and finetuning paradigm [38] optimizes the parameters of the pretrained model  $g_\theta$  and the learnable projection head  $g_\phi$  to maximize the likelihood of predicting labels  $\mathcal{Y}_i$  for the downstream tasks. The paradigm is formally defined as:

$$\theta^*, \phi^* = \arg\max_{\theta, \phi} \sum_{1}^{n} \log P\left(\mathcal{Y}_i | g_{\phi}(g_{\theta}(\mathcal{X}, \mathcal{A}))[i]\right). \tag{1}$$

In contrast, the graph prompt learning paradigm [39], [40] maintains fixed parameters for the pre-trained GNN model. The target of graph promoting is to obtain task-specific graph prompts  $\mathcal{T}$ . Before the optimization of prompt learning, the node embeddings  $\bar{\mathcal{X}}$  and edge embeddings  $\bar{\mathcal{E}}$  of the downstream graphs are initialized by the pre-trained model  $g_{\theta}$ , and the initialization process is formulated as:

$$\bar{\mathcal{X}}, \bar{\mathcal{E}} = g_{\theta}(\mathcal{X}, \mathcal{A}).$$
 (2)

Then, general graph templates will be added to the input graph that include two learnable components, i.e., feature (node-level) prompts and adjacency (edge/motif-level) prompts:

$$\mathcal{G}^*: (\hat{\mathcal{X}}, \hat{\mathcal{E}}) = \mathcal{T}(\bar{\mathcal{X}}, \bar{\mathcal{E}}). \tag{3}$$

To adapt the downstream tasks, the optimization of graph prompting aims at finding the optimal prompt parameters  $\mathcal{T}$  that maximize the likelihood of predicting the correct labels. The optimization process is formally defined as:

$$\mathcal{L} = -\sum_{i=1}^{n} \log P(\mathcal{Y}_i) |\mathcal{G}^*[i]). \tag{4}$$

Both graph prompt learning and conventional pretraining/fine-tuning approaches leverage pre-trained models to optimize downstream task performance. And both methodologies initiate with a model trained on extensive datasets and subsequently adapt it to target specific tasks. While they share a common goal, they approach the task adaptation process in different ways: (1) In the pre-training/fine-tuning paradigm, adaptation to the downstream task is achieved by adjusting the entire model's parameters to better suit the task. While graph prompt learning modifies the input graph data or the way information is processed by the model through prompts. These prompts guide the model to apply its pre-trained knowledge in a way that's beneficial for the task at hand, requiring minimal changes to the model itself. (2) Graph pre-training and finetuning is less flexible and efficient in adapting to new tasks, as it requires a separate fine-tuning phase for each new task, which can be computationally intensive. While graph prompt learning is more efficient in terms of computation and time, as it does not necessitate extensive retraining. It's also more flexible, allowing for quick adaptation to a variety of tasks with simple changes in the prompts. (3) Graph pre-training and fine-tuning requires potentially significant modifications to the model's parameters and structure for different tasks, which can lead to overfitting, especially with small task-specific datasets. While graph prompt learning minimizes the risk of overfitting by keeping the model's parameters largely unchanged, using prompts to direct the model's attention or processing in a task-relevant manner.

# 3.2 Comparision with Graph Few-shot Learning

Few-shot learning focuses on enabling models to learn new tasks with very limited amounts of labeled data, typically referred to as "shots" [41]. Few-shot learning on graphs aims to generalize well on graph-structured data, even when only a few examples of certain nodes, edges, or subgraphs are available for training [42], [43]. To address few-shot learning problems over graphs, meta-learning methods are usually adopted [44]. The application of meta-learning in graph learning involves training a model on various tasks, such that it can leverage prior knowledge from various tasks to rapidly adapt to new, unseen tasks with only a few labeled examples. Specifically using the node classification task as an example, consider a set of tasks  $\mathcal{T} = \{T_1, T_2, ..., T_n\}$  drawn from a distribution over tasks  $p(\mathcal{T})$ . Each task  $T_i$  is associated with a graph  $G_i = (V_i, \mathcal{E}_i)$ , in which  $V_i$  is the set of nodes and  $\mathcal{E}_i$  is the set of edges. Moreover, each task  $T_i$  involves a node classification problem with its own training set  $D_{train}^{i}$ and validation set  $D_{val}^{i}$ . The objective during meta-training is to learn a model  $\mathcal{M}_{\theta}$  that minimizes the loss on  $D_{val}^{i}$  after

being fine-tuned on  $D^i_{train}$ . The meta-learning objective can be formalized as:

$$\mathcal{L} = \sum_{T_i \in \mathcal{T}} \left( D_{\text{val}}^i ; \theta_i' \right),$$
  

$$\theta_i' = \text{Update} \left( \theta, D_{\text{train}}^i \right).$$
(5)

where the Update operation represents the adaptation process (e.g., a few gradient steps), and  $\mathcal L$  denotes the loss objective (e.g., cross-entropy for classification). Then, the adaptation process involves adjusting the model parameters based on a few examples from the new task, leveraging the knowledge gained during the meta-training phase. Specifically, when given a new task  $T_{new}$  with its own graph  $G_{new} = (V_{new}, \mathcal E_{new})$  and a small labeled dataset  $D_{train}^{new}$ , the model  $\mathcal M_\theta$  is firstly fine-tuned on  $D_{train}^{new}$  to obtain adapted parameters  $\theta'_{new}$  and the adapted model  $\mathcal M_{\theta'_{new}}$  can now be evaluated on a separate test set  $D_{test}^{new}$  for the new task.

Graph prompt learning, on the other hand, seeks to repurpose existing models to new tasks through the clever design of prompts, which guide the model's understanding and application of its pre-existing knowledge to the task at hand with minimal data. Unlike meta learning, graph prompt learning does not need to specifically design other models or special learning paradigms to generalize well from a small number of examples.

## 4 DESIGN PRINCIPLE

In this section, we summarize the basic prompt design methodologies for a better understanding of the working principles and mechanisms behind graph prompting. We first summarize the token design principles. Then we sum up the general task alignment mechanisms of the inherent gap between the pre-trained and downstream tasks. Finally, the prompt tuning methods are introduced.

## 4.1 Prompting Tokenization

The concept of tokens is derived from NLP, which is proposed to segment text into meaningful units. The tokens capture the semantic and syntactic structure of the text. Tokenization techniques [45], [46], encompass various levels, including character-level, word-level, subword-level, and sentence-level fragments, etc. By decomposing long texts into smaller, more manageable units, the tokenization process enables language models to process and generate text more efficiently, reducing computational complexity and memory requirements. Graph prompting learning also has learnable tokens designed for graph-structured data, which decomposes complex large graphs into smaller, meaningful subgraphs or graph features, thereby enabling more efficient handling of graphs. Unlike text or sentences, graphstructured data cannot be directly segmented based on spaces or punctuation marks. Based on the information it captures across different levels of graphs, tokenization for prompting learning can be classified into three types, i.e., node tokenization, structure tokenization, and task tokenization.

## 4.1.1 Node Tokenization

During the pretraining phase, the pre-trained model generally adopts an unsupervised loss, which mainly focuses on the structural characteristics of pre-trained large-scale graphs. In this context, the model's ability to adapt to node features is relatively poor, necessitating node-level prompts for rapid adaptation to downstream tasks. Let  $\mathcal{P}_{\text{node}} = \{p_1, p_2, \cdots, p_{|\mathcal{P}_{\text{node}}|}\}$  denote the learnable node-level  $|\mathcal{P}_{\text{node}}|$  prompt tokens, where  $\mathbf{p}_i \in \mathbb{R}^{1 \times d}$  and d denotes the dimensionality of the node features. In practice, we observe  $|\mathcal{P}_{\text{node}}| \ll N$  in graph prompt learning tactics. Based on these token vectors, the node-level tokenization process can be expressed by the following formulation,

$$\hat{\mathbf{x}}_i = \mathbf{x}_i \oplus \left(\mathbf{x}_i \otimes \sum_{k=1}^{|\mathcal{P}|} w_{ik} \mathbf{p}_k\right), \tag{6}$$

where  $\oplus$  generally denotes the add operation,  $\otimes$  denotes the multiplication operation, and  $w_{ik}$  denotes the adaptive weight for different types of nodes. The node tokenization process aims at replacing the input node features  $\mathbf{x}_i$  with the prompted features and sending  $\hat{\mathbf{x}}_i$  for downstream processing.

#### 4.1.2 Structure Tokenization

Many works proved that there is a structural discrepancy between the pretraining and downstream dataset [39], [47], [48]. For example, the graph structure is extremely different between a pertaining citation network and downstream molecular graphs [48]. The molecular graphs are more dense and have a larger average node degree, while the citation graphs have a small node degree. Compared with node tokenization, structure tokenization provides a perspective to capture global information of a target node  $v_i$ . The structure token is also called the semantic or contextual token, as the graph structure always resides and preserves rich selfinformation and contextual information by neighboring node features and connections [49]–[51], which play distinct roles in various downstream tasks. Let p denote a structure-related structure prompt around the center node  $v_i$ , which can be one type of graph meth-paths, motifs, subgraphs, etc [52], [53]. Then the  $\mathcal{P}_{Struc.} = \{\mathbf{p}_1, \mathbf{p}_2, \cdots, \mathbf{p}_{|\mathcal{P}_{Struc.}|}\}$  denotes the set of structure prompts. Let  $\mathbf{z}_i$  denote the node representation of  $v_i$  aggregated with structure information. We summarize the general process based on  $\mathcal{P}_{Struc.}$ ,

$$\mathbf{z}_{i} = \sigma \left( \sum_{j \in \mathcal{N}(i)} \alpha_{i,j} \cdot \mathbf{z}_{j} \right),$$

$$\alpha_{i,j} = \frac{\exp \left( \sigma \left( \mathbf{p}_{i}^{T} \cdot \left[ \mathbf{z}_{i} \otimes \mathbf{z}_{j} \right] \right) \right)}{\sum_{j \in \mathcal{N}(i)} \exp \left( \sigma \left( \mathbf{p}_{i}^{T} \cdot \left[ \mathbf{z}_{i} \otimes \mathbf{z}_{k} \right] \right) \right)},$$
(7)

where  $\otimes$  denotes the multiplication or concatenation operation. GPPT [53] designs subgraph-centered structure prompts based on the social influence theory [54] to leverage the expressive neighborhood information. SAP [55] connects several prompt tokens to the original graph by cross-links. HetGPT [52] proposes the meta-path based structure prompting tokens. IGAP [47] further designs a recessive prompt learning scheme from the spectral space. Inspired by cluster-based graph pooling, SUPT [56] proposes clustering prompts

and node-selection graph pooling prompting scheme, for better representation of graph structures.

## 4.1.3 Task Tokenization

During the pretraining phase, information from downstream tasks is not utilized. To rapidly adapt to the characteristics of downstream tasks and achieve quick fitting for specific scenarios, it is necessary to design task tokens. Task tokens are designed to suit the various downstream tasks. Let  $\mathcal{P}_{\text{task}} = \{p_1, p_2, \cdots, p_{|\mathcal{P}_{\text{task}}|}\}$  denote task-level  $|\mathcal{P}_{\text{task}}|$  prompt tokens. Take the node classification task as an example, let  $|\mathbf{Y}|$  denote the number of node classes, we have  $|\mathcal{P}_{\text{task}}| \leq |\mathbf{Y}|$ . GPPT [53], SGL-PT [57], and GPF [58] adopt the task tokens to align the task gaps for better performance.

# 4.2 Task Alignment Strategies

Task alignment methodologies are proposed to reduce the inherent gap between the pre-trained and downstream tasks. Based on the task levels, they can be classified into node-level and graph-level alignment strategies.

# 4.2.1 Node Level Alignment

Node-level alignment aims to learn node-level and structural/context-level prompts for a node classification task. The alignment process can be summarized into two categories, i.e., cross-entropy-based and graph reconstruction-based. Cross-entropy-based ones are primarily designed to address the gap of node features for node classification tasks, while others are designed to remit the structural gap for link prediction tasks. The general process of these methods can be generally formulated as,

$$\mathcal{L} = -\sum \log(y_i \hat{\mathbf{x}}_i). \tag{8}$$

GPPT [53], ULTRA-DP [59], SAP [55] and DeepGPT [60] are representative cross-entropy-based models. GraphPrompt [39] introduces contrastive learning. VNT [61] and GPF [58] employ learnable perturbations to the input graph to modulate the pre-trained node embeddings. HetGPT [52] employs heterogeneous feature prompts through an attention mechanism for node alignments.

Graph reconstruction-based methods take the link prediction task as the objective, which is in line with the classical learning process of reconstruction loss. Positive nodes  $\{v_i^+\}$  and negative nodes  $\{v_i^-\}$  around a given center node  $v_i$  are randomly sampled, then the triplets the objective is adopted to increase the similarity between graph instance  $v_i$  and  $v_i^+$ , while decreasing that between  $v_i$  and  $v_i^-$ ,

$$\mathcal{L} = -\sum_{(v_i, v_i^+, v_i^-)} \log \frac{\exp(z^p(v_i) \otimes z^p(v_i^+))}{\sum_{v_u \in N(v_i)} \exp(z^p(v_i) \otimes z^p(v_u))}, \quad (9)$$

where  $\otimes$  denotes the similarity measurement,  $N(v_i)$  denotes the k-hop neighbors of  $v_i$ . PGCL [62], SGL-PT [57] are typical models. SGL-PT integrates class-wise prototypes based on Eq. (9) to represent essential features corresponding to labels, which encourages the similarity scores between examples of a class and its corresponding prototype larger than other prototypes. PGCL adds a fusion operation between the graph's semantic and contextual views. In addition, contrastive learning is also adopted to enhance the differentiation.

# 4.2.2 Graph Level Alignment

Graph-level alignment aims to learn graph-level prompts for a graph or subgraph-related classification task. In this context, the objectives of task head tuning and prompt tuning are aligned, and can be formulated as follows:

$$\mathcal{L} = -\sum_{i} \log \frac{\exp(\widetilde{z_{G_i}^p} \otimes z_{Y_i}^p)}{\sum_{c \in Y} \exp(\widetilde{z_{G_i}^p} \otimes z_c^p)}, \tag{10}$$

where  $\otimes$  denotes the similarity measurement,  $(\widetilde{z_{G_i}^p})$  denotes the prompted graph latent representation. Based on this framework, All-in-One [40] proposes graph-level contrastive learning prompting. GPF [58] tunes the prompt token and the task head via maximizing the likelihood of ground truth labels.

# 4.3 Prompt Tuning Strategies

Prompt tuning methods are proposed to reduce the inherent gap between the pre-trained and downstream tasks. Prompt Tuning Methods can be generally categorized into pretext-based and task-oriented methods.

# 4.3.1 Tuning in Line with Pertaining Objectives

If the upstream and downstream tasks and data characteristics are similar, the same loss function used during the pretraining phase can be applied to further optimize the downstream tasks. Take the node classification task as an example, the tuning process can be formalized as,

$$\mathcal{L}_{\text{pretrain}} = -\log P\left(Y_{\text{pretrain}} | F(X_{\text{pretrain}}, E_{\text{pretrain}})\right),$$

$$\mathcal{L}_{\text{tunning}} = -\log P(Y_{\text{down}} | F(X_{\text{down}}, E_{\text{down}},$$

$$\mathcal{P}_{\text{node}}, \mathcal{P}_{\text{structure}}, \mathcal{P}_{\text{task}})),$$
(11)

where F denotes the learnable graph mapping functions, and  $\mathcal{P}$  denotes the learnable prompt templates in tunning processes. They adopt the same F in pertaining process for downstream tunning. GPPT [53] and VNT [61] utilize the same loss objective for both link prediction and node classification tasks. GraphPrompt [39] follows the same node and graph classification objective loss in its pertaining stage. HetGPT [52] and SAP [55] adopt the contrastive loss for nodes to optimize the prompt tokens since their pre-training procedure has the same contrastive task as well. ULTRA-DP [59] designs edge prediction and neighboring prediction loss corresponding with the pre-trained tasks. PRODIGY [63] conducts the neighbor matching constraint in the tunning stage, which is in line with its pre-trained tasks.

#### 4.3.2 Task-oriented Tuning

Due to the significant differences between the objectives of downstream tasks and the unsupervised pretraining objectives, many models have proposed customized task-directed tuning methods. To better adaptation of various tasks, type-specific feature tokens, structure-aware graph tokens, and task-related tokens are designed. In general, these works always adopt the multi-task architecture to capture more complex features and substructures,

$$\mathcal{L} = \mathcal{L}_{\text{node}}(X, \mathcal{P}_{\text{node}}) + \mathcal{L}_{\text{graph}}(X, \mathcal{P}_{\text{structure}}, \mathcal{P}_{\text{task}}),$$
(12)

where  $\mathcal{L}_{node}$  and  $\mathcal{L}_{graph}$  denotes the node-level and graph-level oriented objective functions. Specifically, GPF [64] focus on a graph classification task. Therefore, it requires us to optimize the prompt token and the task head via maximizing the likelihood of ground truth labels based on graph embeddings generated from a pre-trained model. HetGPT enhances feature tokens by enforcing them highly related to different node type, and a multi-view neighborhood aggregation scheme to capture the heterogeneous substructures. SGL-PT [57] proposes multi-task tuning objectives, to address the complex requirements of downstream tasks. All-in-One [40] generates an induced graph for each node, aligning the graph label with the target node label, and considers this graph an individual task.

# 4.4 Homogeneous Graph Prompt

In this section, we will present studies that integrate prompt learning into homogeneous graphs, characterized by having only one type of nodes and edges. As the basis of graph prompt learning, these works focus more on the differences between graphs and other data types, such as non-Euclidean characteristics. The efforts are dedicated to designing pretraining tasks and prompting architectures suitable for graph structures, and proposing relevant optimization methods.

## 4.4.1 Prompting the Input Graph

In the first series of works, prompts are inserted into the original graph data, generating a *prompted graph* which will be fed into the pre-trained GNN model.

VNT [61] inserts a set of virtual nodes into the graph, which function as soft prompts tailored to a few-shot node classification (FSNC) task. The original feature of virtual nodes  $P \in \mathbb{R}^{P \times d}$  are learnable, and are fed into the pretrained Graph Transformer (GT) alongside the real nodes in the graph to generate prompted node representations:

$$[E^{1}||Z^{1}] = GTL^{1}([E^{0}||P]) \in \mathbb{R}^{(V+P)\times d},$$
  
 $[E^{l}||Z^{l}] = GTL^{l}([E^{l-1}||Z^{l-1}]), \quad l = 1, ..., L,$ 
(13)

where V and P respectively represent the number of real nodes and virtual nodes.  $E^0$  is the output of the embedding layer of GT for real nodes, and GTL are GT layers. P are finetuned together with a classifier with cross entropy classification objective. With few parameters to be optimized, these virtual prompted nodes effectively harness the rich knowledge contained in GT, and help push node representations from the same classes closer. To enhance the transferability between FSNC tasks and get more informative prompts, VNT introduces the GPPE module, which utilizes an attention mechanism to gather information from prompts associated with other tasks.

In addition to introducing virtual prompt nodes, All in One [40] further give consideration to the edge connections between nodes. For two virtual nodes, the edge between them are learned adaptively. Specifically, for two virtual nodes, the edge connecting them is learned adaptively. Moreover, the presence of an edge connecting a virtual node and a real node is determined based on their similarity:

$$w_{ik} = \sigma(\boldsymbol{p}_k \cdot \boldsymbol{x}_i^T), \text{if } \sigma(\boldsymbol{p}_k \cdot \boldsymbol{x}_i^T) > \delta,$$
 (14)

where  $\delta$  is a threshold. Then, the feature of real node  $v_i$  is updated with aggregation of virtual nodes:

$$\hat{\boldsymbol{x}}_i = \boldsymbol{x}_i + \sum_{i=1}^P w_{ik} \boldsymbol{p}_k. \tag{15}$$

Prompt tuning is accomplished through a meta-learning mechanism. A similar idea is proposed in PSP [55], which consistently utilize structural information throughout both pre-training and prompt adjustment with class prototype nodes and learnable edges.

# 4.4.2 Prompting the Model Output

While using prompts as graphs is useful for aligning with graph data, this approach can be cumbersome. As a result, another class of methods considers adjusting the output vectors of GNN models to incorporate prompt information.

GPPT [53] consolidates the pre-training and downstream node classification tasks into a unified framework of masked edge prediction. To accomplish this, it introduces two distinct types of prompt tokens: task tokens and structure tokens. Each task token is a vector representing a node label. Meanwhile, the structure token encapsulates k-hop neighborhood information of a node by aggregating the output of the pre-trained GNNs. For prompt tuning, it first generate such token pair for each node and class:

$$f_{prompt}(v_i, y) = [T_{task}(y), T_{structure}(v_i)].$$
 (16)

Subsequently, it undertakes the task of edge prediction for the two tokens, utilizing a cross-entropy classification loss function for optimization.

As GPPT is specifically tailored for node classification, GraphPrompt [39] strives to offer flexibility in adapting to a diverse range of downstream tasks. Recognizing that graph learning tasks can be reframed as subgraph similarity prediction tasks, GraphPrompt adopts the subgraph as its fundamental unit. During the pre-training phase, GNNs are optimized using a link prediction objective, grounded in the assumption that nearby nodes tend to exhibit similar subgraph patterns:

$$\mathcal{L}_{pre} = -\sum_{(v,a,b)\in\mathcal{T}_{pre}} \log \frac{\exp(\operatorname{sim}(\boldsymbol{s}_v, \boldsymbol{s}_a)/\tau)}{\sum_{u\in\{a,b\}} \exp(\operatorname{sim}(\boldsymbol{s}_v, \boldsymbol{s}_u)/\tau)}.$$
(17)

During the fine-tuning stage, to furnish the model with task-specific cues, a tailored prompt  $p_{task}$  is designed for each task:

$$s_{task,\circ} = \text{READOUT}(\{p_{task} \odot h_V : v \in V(\text{Subgraph}_{\circ})\}).$$
(18)

We anticipate that the prompted subgraph representation will exhibit similarity to the class prototype, which is calculated as the average in the k-shot setting. The prompt tuning process is carried out using contrastive learning techniques:

$$\mathcal{L}_{\text{prompt}} = -\sum_{(circ_i, y_i) \in \mathcal{T}_t} \log \frac{\exp(\text{sim}(\boldsymbol{s}_{task, \circ_i}, \tilde{\boldsymbol{s}}_{task, y_i}) / \tau)}{\sum_{c \in Y} exp(\text{sim}(\boldsymbol{s}_{task, \circ_i}, \tilde{\boldsymbol{s}}_{task, c}) \tau)}$$
(19)

To be adaptive to different pre-train tasks, GPF [64] designs a simple yet effective graph prompt by element-wise masking node feature:

$$X = \{x_1, x_2, ..., x_N\},$$
 (20)

$$X^* = \{x_1 + p, x_2 + p, ..., x_N + p\},\$$

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Afterwards, the model is optimized to maximize the classification likelihood. Theoretical analysis demonstrates that such prompts possess the capability to approximate any arbitrary prompting function.

MultiGPrompt [65] also concerns about the pre-train objective designing. Multiple pretext tokens for different pre-train task are introduced to avoid mutual negative influence. Also, tokens are different for different GNN layers, because they focus on different scope of data patterns.

$$\mathcal{T}_{\langle k \rangle} = \{ \boldsymbol{t}_{\langle k \rangle,0}, ..., \boldsymbol{t}_{\langle k \rangle,L} \},$$

$$\boldsymbol{H}^{l+1} = GNN(\boldsymbol{t}_{\langle k \rangle,l} \odot \boldsymbol{H}^{l}, \boldsymbol{A}),$$

$$\boldsymbol{H}_{\langle k \rangle} = \sum_{l=0}^{L} \alpha_{l} \boldsymbol{H}_{t_{\langle k \rangle,l}}$$
(21)

In the adaption phase, composed prompts compose the K pretext tokens together to provide task-specific information. Also, there are open prompts that are directly tuned to provide global pre-train knowledge.

# 4.4.3 Advanced Prompt Design with More Information

The previous two sections introduced some fundamental methods for designing graph prompts. However, due to the complexity of graph data, subsequent works have focused on carefully designing the structure of prompts to introduce information from various aspects, in order to make prompts more informative.

IGAP [47] believes that there are significant differences in node/edge features and the distribution of topological structures among different graphs. The incompatibility of data patterns between pre-training graphs and fine-tuning graphs can result in negative effects of pre-training. Through theoretical derivation, it has been shown that graph pre-training knowledge based on contrastive learning primarily focuses on low-frequency components. Based on this understanding, prompts are proposed at two levels: graph signals and graph filters. Specifically, graph signals serve as prompts for node features, aiming to enhance their representation:

$$\tilde{x}_i = x_i + \sum_j \alpha_j^i p_{s_j}. \tag{22}$$

To bridge the structural gap, the latter prompts focus on aligning the low-frequency components.

$$U_{ft_K} = [v_{ft_1}, ..., v_{ft_k}] \in \mathbb{R}^{M \times K},$$

$$U_{pt_K} = P_t U_{ft_K},$$

$$\tilde{Z} = P_t U_{ft_K} g_{\theta}(\Lambda_{ft}) U_{ft_K}^T P_t^T \tilde{X}.$$
(23)

Furthermore, to address the task type gap, the prompt tokens undergo training with the InfoNCE loss function.

ULTRA-DP [59] focus on the multi-task graph learning scenario, and proposes a unified graph mixing pre-training framework. For task recognition, N pre-train tasks are embedded as a set of trainable vectors  $\{p^{task(1)},...,p^{task(N)}\}$ . Post pre-training, the task-specific semantic knowledge are retained in task embeddings, while the task-independent global knowledge are encapsulated in the GNN. Thereby, the integrity of the pre-training process are well preserved. For

position recognition, the position of each node in the graph are represented by its *t*-reachability to selected anchors:

$$\tilde{\boldsymbol{p}}_{i}^{pos} = (Rch(i, a_{1}, t), Rch(i, a_{2}, t), Rch(i, a_{m}, t)),$$

$$\boldsymbol{p}_{i}^{pos} = \tanh(\boldsymbol{W}^{pos} \frac{\tilde{\boldsymbol{p}}_{i}^{pos}}{\sigma_{i} + \epsilon} + \boldsymbol{b}^{pos}).$$
(24)

For a node  $v_i$  associated with a pre-training task j, the prompt is formulated as the weighted sum of the two embeddings:

$$\boldsymbol{p}_i = \boldsymbol{p}^{task(j)} + w \boldsymbol{p}_i^{pos}. \tag{25}$$

G-Prompt [66] is a graph level prompting method based on graphon. The first key component is the Graph-Level Prompt Generation module (GP) , estimating graph embeddings that encapsulate the knowledge of downstream tasks and produces graph-level prompts according to such knowledge. Then it undergoes prompt integration and optimization steps based on the execution of downstream tasks. Additionally, there is a Graph Answer module (GA) that makes precise forecasts given different graph-level prompts. For every prompt, it estimates the conditional probability of the input sample belonging to a specific class. Subsequently, it determines the prediction by choosing the category with the highest likelihood among all considered categories.

## 4.5 Heterogenous Graph Prompt

The heterogeneous graph [67], [68] typically comprises various types of nodes and edges as well as multi-model attribution with each node. On the one hand, unlike the homogeneous graph, its heterogeneity more effectively captures the complex relationships found in real-world scenarios, including social media graphs, knowledge graphs, and academic networks. On the other hand, this heterogeneity presents numerous challenges when adopting typical homogeneous graph learning techniques. For instance, prompt learning on homogeneous graphs heavily relies on a wellconstructed node embedding space that presupposes uniform node characteristics and interconnections. This assumption simplifies the embedding process but does not hold in heterogeneous graphs. In heterogeneous environments, nodes and edges differ not only in type but often in their attributes and the nature of their connections [69]. As a result, traditional node embedding techniques that work well in homogeneous settings lose their effectiveness because they fail to capture the multifaceted nature of the relationships and interactions [52]. To address these challenges, specialized techniques for heterogeneous graph learning have been developed.

# 4.5.1 Function-based Heterogeneous Graph Prompting

The first series of approaches [52] aims to reformulate the downstream task via a novel graph prompting function to better align with the pretext contrastive task. Formally, given a heterogeneous graph as  $G=(V,E,A,R,\phi,\varphi)$ , where V and E stand for the node and edge sets, respectively. A and B are the type sets of nodes and edges, respectively. They can be identified by the mapping functions B and B0, given as B0 identified by the mapping functions B1. Inspired by the prompt-based learning for NLP tasks and contrastive learning for graph neural network pretraining, the function-based heterogeneous graph prompt focuses on transforming

the input node v and its associated novel class c into a pairwise template, given as:

$$l(v) = [z_v, q_c], \tag{26}$$

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where  $z_v$  and  $q_c$  are the representations of node v and class c, respectively. l(v) is the graph prompting function. After that, this function-based prompt learning framework can be optimized by maximizing the mutual information between node-node or node-graph pairs.

**Virtual Class Token:** Equation 26 gives an overall perspective of the function-based heterogeneous graph prompt. For shifting the paradigm from traditional node classification via this approach, HetGPT proposed a virtual class prompt, which serves as a dynamic proxy for each class and bridges the gap between the node embeddings and the class labels. Formally, the set of virtual class tokens *Q* can be defined as:

$$Q = \{q_1, q_2, \dots, q_C\},\tag{27}$$

where C is the total number of classes in A. In detail, each virtual class token is a trainable vector with the same dimension as the node embedding. To initialize the representation of each token, HetGPT utilized a simple but effective way:

$$q_c = \frac{1}{N_c} \sum_{v \in V_L, y_c = c} h_v, \forall c \in \{1, 2, \dots C\},$$
 (28)

where  $N_c$  is the number of nodes of class c, let  $V_L$  mark the labeled node set in the target domain when dealing with a semi-supervised task.

**Heterogeneous Feature Prompt:** Another shift is to align the feature space from the pre-training graph to the prompted graph. Formally, the prompt tokens of each feature type can be defined as:

$$F = \{F_a | a \in A\}, F_a = \{f_1^a, f_2^a, \dots, f_K^a\},$$
 (29)

where K is an adjustable hyperparameter for different datasets. Then, the node feature  $x_i^a$  can be prompted through the feature token  $f_i^a$ :

$$\tilde{x}_{i}^{a} = x_{i}^{a} + \sum_{k=1}^{K} w_{i,k}^{a} \cdot f_{k}^{a},$$

$$w_{i,k}^{a} = \frac{\exp(\sigma((f_{k}^{a})^{T} \cdot x_{i}^{a}))}{\sum_{j=1}^{K} \exp(\sigma((f_{j}^{a})^{T} \cdot x_{i}^{a}))},$$
(30)

where  $w_{i,k}^a$  is the attention weight, and  $\sigma(\cdot)$  is the activation function.  $\tilde{x}_i^a$  is the prompted node feature. Then the node embedding H can be obtained by passing through the pre-trained graph modeling method.

**Multi-View Aggregation:** Due to the heterogeneity of the prompted graph, there are two ways to aggregate the node embeddings. The first way is type-based aggregation via a two-level attention mechanism [70] for enhancing the local information. For each node with M different connected node types  $a_1, a_2, \ldots, a_M$ , the type-specific fused information for node i can be obtained from the neighbor set  $\mathcal{N}i^{a_m}$ :

$$h_{i}^{a_{m}} = \sigma \left( \sum_{j \in \mathcal{N}_{i}^{a_{m}} \cup \{i\}} \alpha_{i,j}^{a_{m}} \cdot \tilde{h}_{j} \right),$$

$$\alpha_{i,j}^{a_{m}} = \frac{\exp(\sigma(\mathbf{a}_{a_{m}}^{\mathrm{T}} \cdot [\tilde{h}_{i} \parallel \tilde{h}_{j}]))}{\sum_{k \in \mathcal{N}_{i}^{a_{m}} \cup \{i\}} \exp(\sigma(\mathbf{a}_{a_{m}}^{\mathrm{T}} \cdot [\tilde{h}_{i} \parallel \tilde{h}_{k}]))},$$
(31)

where  $\parallel$  denotes the concatenation operation.  $\mathbf{a}_{a_m}$  is the type-specific node attention vector.  $\tilde{h_i} \in \tilde{H}$  is the prompted node embedding for node i. Let aTP be the type-based semantic attention vector. Then, all type-specific representations can be fed through semantic attention:

$$z_{i}^{\text{TP}} = \sum_{i=1}^{M} \beta_{a_{m}} \cdot h_{i}^{a_{m}}, \beta_{a_{m}} = \frac{\exp(w_{a_{m}})}{\sum_{k=1}^{M} \exp(w_{a_{k}})},$$

$$w_{a_{m}} = \frac{1}{|V_{T}|} \sum_{i \in V_{T}} \mathbf{a}_{\text{TP}}^{\text{T}} \cdot \tanh(W_{\text{TP}} \cdot h_{i}^{a_{m}} + b_{\text{TP}}),$$
(32)

where  $W_{\rm TP}$  is the weight matrix, and  $b_{\rm TP}$  is the bias vector.

Another aggregation strategy is metapath-based aggregation. Given a set of metapaths  $P_1, P_2, \dots, P_N$ , the information can be aggregated via node attention:

$$h_{i}^{P_{n}} = \sigma \left( \sum_{j \in \mathcal{N}_{i}^{P_{n}} \cup \{i\}} \alpha_{i,j}^{P_{n}} \cdot \tilde{h}_{i} \right),$$

$$\alpha_{i,j}^{P_{n}} = \frac{\exp(\sigma(\mathbf{a}_{P_{n}}^{\mathbf{T}} \cdot [\tilde{h}_{i} \parallel \tilde{h}_{j}]))}{\sum_{k \in \mathcal{N}_{i}^{P_{n}} \cup \{i\}} \exp(\sigma(\mathbf{a}_{P_{n}}^{\mathbf{T}} \cdot [\tilde{h}_{i} \parallel \tilde{h}_{k}]))},$$
(33)

where  $\mathbf{a}_{P_n}$  is the path-specific node attention vector for metapath  $P_n$ . Then, node i's global structural information  $z_i^{\mathrm{MP}}$  can be obtained through each metapath, defined by:

$$z_{i}^{\text{MP}} = \sum_{i=1}^{M} \beta_{P_{n}} \cdot h_{i}^{P_{n}}, \beta_{P_{n}} = \frac{\exp(w_{P_{n}})}{\sum_{k=1}^{M} \exp(w_{a_{k}})},$$

$$w_{P_{n}} = \frac{1}{|V_{T}|} \sum_{i \in V_{T}} \mathbf{a}_{\text{MP}}^{\text{T}} \cdot \tanh(W_{\text{MP}} \cdot h_{i}^{P_{n}} + b_{\text{MP}}),$$
(34)

where  $W_{\rm MP}$  and  $b_{\rm MP}$  follow the similar definition as in Equation 32. Finally, all information from the two methods can be aggregated by:

$$z_i = \sigma(W[z_i^{MP} \parallel z_i^{TP}] + b),$$
 (35)

where W and b are the weight matrix and bias vector, respectively.

**Learning and Inference:** For training the whole pipeline, we can follow the Equation 26. Formally, the InfoNCE [71] loss can be defined as:

$$z'_{v} = \text{MLP}(z_{v}), q'_{c} = \text{MLP}(q_{c}),$$

$$\mathcal{L} = -\sum_{v \in V_{L}} \log \left( \frac{\exp(\text{sim}(z'_{v}, q'_{y_{v}})/\tau}{\sum_{c=1}^{C} \exp(\text{sim}(z'_{v}, q'_{c})/\tau} \right),$$
(36)

For inference on the unlabeled data  $V_U$  with the prompt component, the prediction probability of node v belonging to class c is given by:

$$P(y_c = c) = \frac{\exp(\sin(z_v', q_c'))}{\sum_{k=1}^{C} \exp(\sin(z_v', q_k'))}$$
(37)

# 4.5.2 Template-based Heterogeneous Graph Prompting

Another approach [72] aims to unify the heterogeneity of the input graphs via multiple homogeneous graphs.

**Graph Template:** In detail, a heterogeneous graph can be extracted into multiple homogeneous subgraphs  $G^i = (V^i, E^i)$ , where the node and edge set can be defined as:

$$V^{i} = \{ v \in V | \phi(v) = i \}, E^{i} = \{ (a, b) \in E | a \in V^{i} \land b \in V^{i} \}.$$
 (38)

To preserve the full topology, a homogeneous graph  $G^0 = \{V, E\}$  will be added to the graph template, defined as:

$$\mathcal{GT}(G) = \{G^0\} \cup \{G^i : i \in A\}$$
 (39)

**Task Template:** Following the strategy in this work [39], for each node v, its related  $\delta$ -hop subgraph  $S_v$  can be extract by breadth-first search. Then, the embedding vector of the subgraph  $S_v$  can be individually readout and aggregated by:

$$s_v = \operatorname{AGG}(\{\operatorname{READOUT}(S_v^i) | S_v^i \in \mathcal{GT}(S_v)\}),$$
  

$$\operatorname{READOUT}(S) = \operatorname{AGG}_2(\{h_v : v \in V(S)\}).$$
(40)

After that, three tasks on the graph could be transformed as predicting the similarity scores between the extracted (sub)graph embeddings. For pretraining the model, we can use link prediction task by modeling the large-scale graph data in a self-supervision manner. The pretrain loss is defined as:

$$\mathcal{L} = -\sum_{v,a,b \in \mathcal{D}_{pre}} \log \left( \frac{\exp(\sin(s_v, s_a)/\tau)}{\sum_{u \in \{a,b\}} \exp(\sin(s_v, s_u)/\tau)} \right), \quad (41)$$

where  $\mathcal{D}_{pre}$  is the pre-constructed triplet dataset.

**Template-based Dual-prompting Tune:** To advance the prompt learning on the heterogeneous graph, we need to consider the prompt for feature and heterogeneity. The feature prompt  $\mathbf{p}^{feat}$  can be defined as the readout layer for some subgraph S:

READOUT(
$$\{\mathbf{p}^{feat} \odot h_v | v \in V(S)\}$$
), (42)

where  $\odot$  denotes the element-wise multiplication. The heterogeneity prompt should capture multi-facets across different tasks. For a specific task, its task-specific learnable heterogeneity prompt of each subgraph in the graph template can be defined as  $\mathbf{p}^{het} = (p_0^{het}, p_1^{het}, \dots, p_{|A|}^{het})$ . With those tokens, the aggregation layer can be defined as:

$$AGG(\{(1+p_i^{het}) \odot READOUT(S^i) | S^i \in \mathcal{GT}(S)\})$$
 (43)

For prompt tuning, we can use the labeled training set  $\mathcal{D}_{down}$  by following the same graph similarity manner:

$$\mathcal{L}(\mathbf{p}^{feat}, \mathbf{p}^{het}) = -\sum \log \left( \frac{\exp(\operatorname{sim}(s_{x_i}, \tilde{s}_{y_i})/\tau}{\sum_{c \in Y} \exp(\operatorname{sim}(s_{x_i}, \tilde{s}_c)/\tau} \right). \tag{44}$$

The subgraph and class embedding  $s_{x_i}$  and  $\tilde{s}_c$  are generated based on the prompt vectors  $\mathbf{p}^{feat}$  and  $\mathbf{p}^{het}$ .

## 5 APPLICATIONS

In this section, we summarize the application scenarios of graph prompt learning. Until now, its downstream applications have been primarily confined to molecular graphs, text-attributed graphs, and recommendation systems.

## 5.1 Graph Prompting for Molecules

Molecular Representation Learning plays a crucial role in various natural science fields such as quantitative chemistry, drug discovery, and cell biology. Informative molecular representations can accurately predict molecular properties and their interactions, thereby serving a wide range of practical applications. The chemical structure of molecules inherently forms a graph, with different types of atoms as

nodes and chemical bonds as edges. Consequently, numerous Graph Neural Network models have been designed to extract meaningful molecular representations [73]–[75]. However, directly using task-specific GNN models in real-world applications has significant limitations. These models heavily rely on the quantity and quality of labeled data. In many specific biochemical scenarios, molecular-related labels must be obtained through wet lab experiments, which are expensive and time-consuming. Additionally, the available data often represents only a small fraction of the entire molecular space [76], leading to severe specificity issues. Moreover, the datasets themselves also suffer from label distribution imbalances.

To address these challenges, recent molecular graph research [36], [77], [78] favors the "pretrain, fine-tune" paradigm. This approach involves pretraining on largescale, easily accessible unlabeled data to compensate for GNN models' dependence on labeled data. Generally, GNN pretraining models for Molecular Representation Learning can be divided into two types: 1) Contrastive Learning: Pretrained GNN models aim to maximize the similarity between the target molecular graph and its augmented versions (e.g., masking some nodes). 2) Node Masking: Given a molecular graph, a certain proportion of nodes are masked, and the remaining graph structure is used to predict the types of the masked atoms. Despite the success of GNN models based on the "pretrain, fine-tune" paradigm, they still face some issues. 1) While pretraining helps models capture general molecular structural patterns, it fails to capture information contained in inherent structural patterns (subgraphs). Unlike networks in other domains, many molecular properties are influenced by fixed structural patterns (e.g., motifs, functional groups) that play similar roles or possess similar attributes across different molecules [48], [79]. For example, a benzene ring, composed of six carbon atoms in a ring structure, imparts aromaticity to a molecule and is a crucial structural unit in many organic compounds. 2) For the "pretrain, fine-tune" approach to be effective, the objectives of pretraining and downstream tasks must align; otherwise, negative transfer can occur [80], necessitating more precise engineering design.

To address these issues, the "pre-train, prompt, fine-tune" paradigm might be more suitable. Researchers can design prompts flexibly from the perspectives of atoms (nodes), molecules (graphs), and downstream tasks to bridge the gap between pretraining and downstream tasks. Additionally, prompts can be specifically designed for motifs to explicitly model these fixed subgraph patterns.

## 5.1.1 Graph Prompting for Molecule Property Prediction

Molecular Property Prediction is a graph-level classification task aimed at learning effective molecular representations and mapping them to their respective labels. MolCPT [48] introduces a versatile Graph Motif Prompting framework suitable for both of the aforementioned GNN pretraining methods. MolCPT designs a lookup table for common molecular motifs and initializes it with embeddings output by a pretrained GNN model for these motifs. Given a molecular structure, MolCPT first extracts the common molecular motifs it contains. Then, using Cross Attention, it aggregates the original molecular graph with the extracted motifs to obtain the motif prompt embedding. Additionally,

for the classification task, MolCPT designs k answer vectors as Task Tokens, where k is the number of classification labels. By calculating the inner product similarity between the motif prompt embedding and the Task Token embeddings, the predicted results are output. MolCPT guides the model's focus on molecular motifs through the use of prompts. Its plug-in prompt design approach makes it a classic example of Graph Prompting for molecular property prediction.

# 5.1.2 Graph Prompting for Drug-Drug Interaction

Drug-Drug Interaction (DDI) Event Prediction is a prediction task of the interactions between molecules. Understanding the combined effects of drugs is crucial for treating complex diseases [81]. However, different drug combinations can sometimes have adverse effects [82], reduce each other's efficacy, or even produce toxicity. Therefore, accurate prediction of DDI is essential for combinatorial drug research. DDI can also be viewed as a mathematical problem on a graph, where drugs are nodes and their interactions are edges. Then the DDI prediction problem can be abstracted as an edge classification issue.

DDIPrompt [83] is the first approach to tackle issues in the drug domain using Graph Prompt Tuning. During the pre-training phase, DDIPrompt first constructs a graph based on the chemical structure of molecules (atoms as nodes and bonds as edges) and designs a GNN model that uses graph contrastive learning for the first stage of pre-training. Secondly, DDIPrompt builds a new graph based on Drug-Drug Interactions (drugs as nodes and interactions as edges) and designs another GNN for link prediction in the second stage of pre-training. This hierarchical pre-training allows DDIPrompt to capture both molecular structure information and molecular interaction information simultaneously. In the prompt tuning phase, DDIPrompt designs k answer vectors as Task Tokens based on the classification target, where k is the number of possible DDI relationships. By calculating the similarity between the edge embeddings and Task Token embeddings, DDIPrompt outputs the predicted results. Through hierarchical pre-training and prompt tuning, DDIPrompt effectively alleviates the issue of extremely imbalanced data distribution in DDI downstream task datasets, providing a successful demonstration of applying Graph Prompting to this field.

## 5.2 Prompt Learning on Text-Attributed Graphs (TAGs)

In the realm of data science and artificial intelligence, integrating different types of data modalities is a key challenge. Research on combining text and graphs has emerged as a significant area of focus. Traditionally, text data is represented linearly, while graphs exist in nonlinear structures. In the real world, many datasets not only contain textual information but also embed complex relationships in graphical form. Bridging these modalities is crucial for advancing general artificial intelligence. Currently, research on text and graph integration is in its early stages but shows immense potential. Particularly in the study of text-attributed graphs, blending textual information with graphical structures helps capture complex real-world relationships and semantic information more effectively. For instance, in social networks, user interactions can be represented as graph structures, with

personal information and posts serving as textual attributes. This integration not only enhances data description but also improves analytical capabilities. The rapid development of large language models(LLMs) has provided powerful tools for advancing text and graph integration research. These models better handle and understand relationships between text and graphs, leading to breakthroughs in the field of text-attributed graphs.

An effective way to enhance graph learning is by integrating LLMs with traditional GNNs. While GNNs excel at capturing structural details, they mainly use semantic embeddings as node features, which restricts their capacity to capture the full complexity of nodes. Conversely, while LLMs excel at encoding text, they frequently have difficulty handling the structural complexities inherent in graph data. By combining LLMs with GNNs, the latter can utilize more powerful node features to effectively capture subtle structural differences and contextual clues. This combination harnesses LLMs' strong text comprehension and GNNs' capability to model structural relationships, resulting in more effective and resilient graph learning approaches. Introducing prompt learning into this framework can further enhance the integration of text and graphs. Prompt learning involves using predefined or dynamically generated prompts to guide the model in processing data. In the context of TAGs, prompt learning can help the model make better use of the textual information associated with each node. By focusing on relevant parts of the text, the model can improve tasks such as node classification and link prediction.

The integration of LLMs and traditional GNNs, enhanced by prompt learning, can be categorized into two approaches: LLM-Enhanced Prompting, which uses LLMs to generate prompts that aid GNNs in improving their classification performance, and LLM-Predictive Prompting, which utilizs input graph structures for predictions. By leveraging prompt learning, LLMs can generate more effective prompts that guide GNNs in capturing intricate relationships between nodes and their textual attributes.

# 5.2.1 LLM-Enhanced Graph Prompting

LLM-Enhanced Prompting involves leveraging their powerful capabilities to improve the quality of node embeddings. The resulting embeddings are then incorporated into the graph structure for use by any GNN or directly input into downstream classifiers to perform various tasks.

**Embedding-based Enhancement.** Embedding-based enhancement methods directly use text embeddings generated by LLMs to initialize node features in GNNs, incorporating rich semantic information to improve the model's performance:

$$X_i = f_{LLM}(t_i),$$
  

$$H = f_{GNN}(X, A).$$
(45)

The original text attributes  $t_i$  are transformed into initial node embeddings  $X_i \in \mathbb{R}^D$  and  $X \in \mathbb{R}^{N \times D}$ , in which N is the number of nodes and D is the embedding dimension. These initial embeddings are enhanced using an embedding matrix and adjacency matrix  $A \in \mathbb{R}^{N \times N}$  through Graph Neural Networks (GNNs) to derive node representations  $H \in \mathbb{R}^{N \times d}$ , where d is the dimension of the representations. This approach relies on embedding-visible or open-source

LLMs, enabling direct access to text embeddings and the refinement of LLMs using structural information. G-Prompt [84] optimizes graph PTMs for downstream tasks by generating task-specific graph-level prompts using graphons, optimizing prompt adaptability, and enhancing prediction accuracy through prompt ensembling. OFA [39] uses textattributed graphs to integrate natural language descriptions of nodes and edges, embedding them into a shared space using language models. It introduces nodes-of-interest for task standardization and a novel graph prompting paradigm for contextual learning without fine-tuning. GIMLET [85] integrates language models for TAGs, enhancing generalization and performance in zero-shot molecule property prediction by encoding graph structures and instructions without additional modules. GAugLLM [86] leverages large language models to augment text-attributed graphs by generating enhanced node features and improving edge augmentation, thereby significantly boosting the performance of graph contrastive methods, generative models, and graph neural networks.

**Explanation-based Enhancement.** Explanation-based enhancement methods leverage the strong zero-shot capabilities of LLMs to capture higher-level information, enriching textual attributes. These methods prompt LLMs to generate semantically rich additional information, such as explanations, knowledge entities, and pseudo labels. This generated content can effectively supplement the original data, improving the model's performance. The typical process is as follows:

$$e_i = f_{LLM}(t_i, p), \quad X_i = f_{LLM}(e_i, t_i),$$
  
 $H = f_{GNN}(X, A),$  (46)

where p represents the designed textual prompts and  $e_i$ denotes the additional textual output generated by the LLMs. TAPE [88] is a pioneering work in explanationbased enhancement. It uses LLMs to generate explanations and pseudo labels as prompts to enrich textual attributes. Then, smaller language models are fine-tuned on this basis, and the resulting semantic information is used as initial node embeddings in TAGs. LLMRec [89] improves recommendation systems by utilizing large language models to augment interaction graphs, enhancing user-item interaction edges, item attribute comprehension, and user profiling. This method effectively tackles challenges of data sparsity and low-quality side information, with robustification techniques ensuring high-quality augmentations. DGTL [90] enhances large language models' reasoning and prediction capabilities for text-attributed graphs by integrating graph structure information through tailored disentangled GNN layers, improving performance and interpretability while operating with frozen pre-trained LLMs to reduce computational costs.

## 5.2.2 LLM-Predictive Graph Prompting

Due to the diverse definitions of structure and features across different graphs, direct conversion of graph data into sequential text is often problematic. This complicates the integration of LLMs with graph modalities. Consequently, methods have emerged that utilize LLMs within a unified generative paradigm to predict various graph-related tasks, including classification and inference.

<b>Evaluation Purpose</b>	Metrics	Source				
Overall Performance	Acc Acc, F1, AUC MicroF, MacroF	GPPT [53], PGCL [62], PRODIGY [87], GraphPrompt [39] All-in-One [40] HGPrompt [72]				
Efficiency	#. parameters #. FLOPs	GraphPrompt [39], PGCL [62], HGPrompt [72]				
Flexibility	Error Bound MicroF, MacroF	All-in-One [40] HGPrompt [72]				
Transferability Acc, F1, AUC		All-in-One [40]				

TABLE 1: Evaluation criteria for downstream tasks.

**Flatten-based Prediction.** Flatten-based Prediction is a strategy that flattens the graph into a text format, allowing LLMs to process graph data as if it were a text sequence. This approach typically involves two steps: (1) Using a flattening function  $\operatorname{Flat}(\cdot)$  to convert the graph structure into a sequence of tokens or nodes  $G_{\operatorname{seq}}$ . (2) Applying a parsing function  $\operatorname{Parse}(\cdot)$  to retrieve the predicted labels from the output generated by the LLM. The specific process is as follows:

$$G_{\text{seq}} = \text{Flat}(V, E, T, J),$$
  

$$Y = \text{Parse}(f_{LLM}(G_{\text{seq}}, p)),$$
(47)

where T dentoes the node text attributes, and J for the edge text attributes. p denotes the instruction prompt for the graph task, and Y represents the predicted label. For example, recent works [91], [92] control the output format of LLMs by offering choices and adding instructions in prompts during zero-shot scenarios. GIMLET [85] integrates language models to embed graph structures as well as textual instructions for molecular tasks, enhancing generalization and achieving strong instruction-based zero-shot performance. Instruct-GLM [93] uses natural language instructions to fine-tune LLMs for graph learning tasks, surpassing competitive GNN baselines on datasets like ogbn-arxiv, Cora, and PubMed. **GNN-based Prediction.** GNN-based prediction fully utilizes the advantages of GNNs by integrating the inherent structural features and dependencies in graph data with LLMs,

thereby enabling LLMs to possess structural awareness:

$$H = f_{GNN}(X, A),$$
  

$$\tilde{Y} = \text{Parse}(f_{LLM}(H, p)),$$
(48)

where H denotes the structure-aware embeddings associated with the graph. Extracting outputs from LLMs in this context relies on a parser. However, integrating GNN representations into LLMs typically involves tuning, which facilitates standardizing LLM prediction formats through controlled outputs during training. Several approaches have been suggested to integrate the structural patterns learned by GNNs with the contextual information captured by LLMs. For instance, GIT-Mol [94] integrates Graph, Image, and Text information for advancing molecular science applications. GraphLLM [95] integrates graph learning models with LLMs to enhance their capacity in understanding and reasoning on graph data,

## 5.3 Graph Prompting on Recommendation Systems

In the context of Recommender Systems (RS), elements such as users, items, and attributes are closely interconnected,

interacting through various relationships. This inherent complexity of the data requires that we consider the intricate relationships between entities when devising recommendation strategies. Graph Neural Networks (GNNs), with their exceptional ability to learn complex relationships, have become a powerful tool in the domain of recommender systems [96], [97]. They have shown outstanding performance in enhancing personalized recommendations, increasing user engagement, and improving conversion rates. However, GNN-based recommender systems heavily rely on historical training data, which presents several challenges. Firstly, when historical data is insufficient, the model's predictive performance may be limited. Secondly, if the relationships between users and items change in the future, or if new item categories emerge, models relying on historical data may not adapt well to these changes, thus affecting recommendation quality. Additionally, unstructured text data, such as user reviews and product descriptions, although rich in information, are difficult to leverage effectively by traditional graph

Against this backdrop, Graph Prompt Tuning has emerged as a new solution to address these challenges in recommender systems. It enhances the adaptability and flexibility of GNNs by introducing adjustable prompts. These prompts serve as guidance signals for the model when processing new data, helping it adapt quickly to new user-item interaction patterns and changing relationship structures without much retraining or finetuning. In view of task scenario, we can devide graph prompt tuning-based recommender systems into two categories: streaming recommendation and session-based recommendation.

# 5.3.1 Graph Prompt Tuning for Streaming Recommendation

Graph prompt tuning for streaming recommendation systems arises from the need to adapt quickly and efficiently to rapidly changing user-item interactions that are characteristic of streaming environments. Traditional models often struggle to balance the influx of new data while preserving relevant historical interactions, which can significantly affect the recommendation quality. These approaches uses graph prompt tuning to segment user-item interaction graph into multiple views, allowing the models to focus on specific aspects of data more effectively. This kind of method enhances the adaptability of the system, ensuring that it can respond dynamically to new user preferences and maintain accuracy over time.

GPT4Rec [98] presents a graph prompt tuning methodology designed to improve the adaptability of streaming

recommendation systems to dynamically changing user-item interactions. This approach focuses on disentangling the interaction graph into multiple views to better manage varying aspects of data, which enhances the system's responsiveness to shifts in user preferences and item attributes. Central to this methodology are graph prompts—modular adaptations strategically applied at different levels of the graph structure. These include the following three types of prompts.

**Node-level prompt**. It adjusts attributes or properties of individual nodes, and enhances the model's responsiveness to changes in user or item characteristics. This is mathematically represented as:

$$\tilde{x}_{i} = \tilde{x}_{i} + \sum_{j}^{L} \alpha_{ij} p_{j},$$

$$\alpha_{ij} = \frac{\exp(\tilde{x}_{i} p_{j})}{\sum_{r} \exp(\tilde{x}_{i} p_{r})},$$
(49)

where  $\tilde{x}_i$  is the current data point,  $\alpha_{ij}$  is the weight for prompt j.

**Structure-level prompts**. They address the broader connectivity patterns within the graph, and help the model adapt to structural changes and maintain its interpretative consistency over time:

$$\tilde{x}_{i} = \tilde{x}_{i} + \sum_{j \in N(x_{i})} \beta_{ij} u_{ij},$$

$$\beta_{ij} = \frac{\exp(\tilde{x}_{i} u_{ij})}{\sum_{r} \tilde{x}_{i} u_{ir}},$$

$$u_{ij} = \sum_{k=1}^{K} att_{ij,k} q_{k},$$

$$att_{ij,k} = \frac{\exp(a(\tilde{x}_{i} || \tilde{x}_{j}) q_{k})}{\sum_{r} \exp(a(\tilde{x}_{i} || \tilde{x}_{j}) q_{r})},$$
(50)

Here  $x_i$  and  $x_j$  are current data points for adjacent nodes, and a is the linear mapping.

**View-level prompts**. This is used to aggregate insights from the disentangled views, for ensuring a comprehensive and coherent interpretation of the graph. This view centers on updating a small set of 'codebook' prompts  $J = [j_1, \cdots, j_n]$ , rather than relearning the entire model's parameters.

$$\hat{x}_{i} = \operatorname{Atten}(\operatorname{prompt}(x_{i}), [\tilde{x}_{i,1}, ..., \tilde{x}_{i,n}]) = x_{i} + \sum_{j} \epsilon_{i,j} \tilde{x}_{i,j},$$

$$\epsilon_{i,j} = \frac{\exp(\operatorname{prompt}(x_{i})\tilde{x}_{i,j})}{\sum_{r} \exp(\operatorname{prompt}(x_{i})\tilde{x}_{i,r})} = \frac{\exp(p(x_{i}+j)\tilde{x}_{i,j})}{\sum_{r} \exp(p(x_{i}+j)\tilde{x}_{i,r})},$$
(51)

By integrating these prompts into the model, GPT4Rec not only adapts more effectively to real-time data streams but also maintains an essential continuity with historical user-item interactions. This balance is crucial for streaming recommendation systems where both current relevance and historical accuracy are needed to enhance user satisfaction and engagement.

## 5.3.2 Session-based Recommendation

For session-based recommendation systems, the target is to harness the rich semantic information contained within textual data alongside the structured interaction data. In session-based contexts, where the graph structure of user interactions provides a natural framework for recommendation, the challenge lies in effectively incorporating the nuanced, unstructured textual descriptions that accompany items and user interactions. By embedding LLMs and prompts into this framework, the proposed methods see to deepen the understanding of user preferences and enhance the recommendation process, tapping into both textual and graphical information for more informed and relevant suggestions.

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LLMGR [99] combines Large Language Models (LLMs) with GNNs, aiming to enhance the performance of session-based recommendation systems. It leverages the powerful natural language processing capabilities of language models, with carefully designed prompt mechanisms, to parse and understand graph-structured data. At the same time, the model processes complex user-item relationship graphs through GNNs, achieving efficient information integration and recommendations. This method particularly emphasizes how to effectively combine text content with graphical representations of user interactions in session data, to capture subtle changes in user behavior and generate more accurate recommendation results.

# 6 BENCHMARK DATASETS AND EVALUATION METH-ODS

In this section, we summarize commonly used datasets and evaluation criteria in graph prompt learning works.

#### 6.1 Evaluation Criteria

We review evaluation methods in experimental sections of representative papers focusing on three major tasks: node classification, graph classification, and link prediction. Accuracy is the most used metric for evaluating both models and their performance, with other additional evaluation methods.

For **Node Classification Tasks**, comparisons are made between state-of-the-art approaches to evaluate the model or learning framework performance. When comparing against the baseline, two-thirds of the papers only select accuracy as the evaluation metric. While other papers incorporate other metrics including F1-scores, AUC score(Area Under the Curve), Micro-F and Macro-F to provide a more comprehensive assessment.

For **Link Prediction Tasks**, the primary metrics used are AUC and AP (Average Precision), offering a refined measurement of model performance against other state-of-the-art approaches [101]–[103].

For **Graph Classification Tasks**, the evaluation methods and experimentations are relatively less extensive in the graph classification task. Similar to node classification, accuracy serves as the chief metric when compared to other state-of-the-art approaches in graph classification tasks. Some papers also further analyze flexibility, parameter efficiency, and other factors using similar metrics as those used in node classification.

For **Model Analyses**, current works conduct the transferability evaluation, flexibility evaluation, and efficiency evaluation tasks. *Transferability Analysis*. Accuracy, F1-score, and AUC score are utilized in experiments as metrics. *Flexibility Analysis*. Some papers use accuracy as metric in flexibility analysis, while others use error bounds to assess. *Efficiency* 

TABLE 2: Detailed summarization of homogeneous graph datasets.

Domains	Dataset	#. Graphs	#. Classes	#. Nodes	#. Edges	#. Feature	Task Type	Source
Citation Networks	Cora	1	7	2708	5429	1433	N & L	GPPT [53], All-in-One [40], PGCL [62]
	Citeseer	1	6	3,327	4732	3703	N & L	GPPT [53], All-in-One [40], PGCL [62]
	PubMed	1	3	19,717	44338	500	N & L	GPPT [53], All-in-One [40], PGCL [62]
	CoraFull	1	70	19,793	126,84	126,84	N	GPPT [53]
	ogbn-arxiv	1	40	169,343	1,166,243	128	N	GPPT [53], PRODIGY [87]
	DBLP	1	-	-	-	-	N & L	PGCL [62]
Social Networks	Reddit	1	41	232,965	114,615,873	602	N	All-in-One [40]
	REDDIT-BINARY	2000	2	429.63	497.75	-	G	GNN [100], SGL-PT1 [57]
	REDDIT-MULTI-5K	4999	5	508.52	594.87	-	G	GNN [100]
	REDDIT-MULTI-12K	11929	11	391.41	456.89	-	G	SGL-PT1 [57]
	Flickr	1	-	89,250	899,756	500	N	GraphPrompt [39]
	COLLAB	5000	3	74.49	2457.78	-	G & L	SGL-PT1 [57], OGB [26]
Biological Networks	PROTEINS	1,113	2	39.06	72.82	1	G	GraphPrompt [39], PGCL [62], SGL-PT1 [57], OGB [26]
	COX2	467	2	41.22	43.45	3	G	GraphPrompt [39], PGCL [62]
	<b>ENZYMES</b>	600	6	32.63	62.14	18	G	GraphPrompt [39], PGCL [62]
	BZR	405	2	35.75	38.36	3	G	GraphPrompt [39], PGCL [62]

*Analysis.* This includes parameter efficiency measured by the number of parameters and the number of floating point operations (FLOPs), and fine-tune efficiency, which considers both accuracy and training loss as metrics. Detailed information is provided in Table 1.

We found that papers categorize evaluation approaches differently. In the node classification task, some papers categorize approaches into supervised, pre-trained, joint, and prompt methods, while others into end-to-end GNN, pre-trained, and prompt methods. The supervised methods and end-to-end GNN methods are categorized differently but mostly overlap because of both training a GNN model. These methods include GraphSAGE, GCN, and GAT. Pre-trained methods include methods like Pre-Edge, Pre-DGI, GAE, and GraphCL. GPPT, GraphPrompt, PGCL are the most used prompt methods. In graph classification tasks, approaches are categorized into supervised methods, self-supervised methods, pre-trained methods, and graph kernel methods, using methods similar to those in node classification tasks.

# 6.2 Benchmark Datasets

## 6.2.1 Homogeneous Datasets

There is only one type of nodes and edges in homogeneous graphs. We classify these datasets into four main domains: citation networks, social networks, molecular graphs, and biological graphs. Despite the data structures of molecular graphs and biological graphs are heterogeneous, they are simplified as homophilous graphs for experimentation purposes in papers on graph prompt learning, thus falling under the category of homogeneous graph tasks. Detailed information is provided in Table 2. Compared with other datasets, the size of citation networks and social networks tends to be relatively larger. When the downstream task is node classification, it is typically concentrated in the citation network domain, with the number of nodes ranging from  $10^3$  to  $10^6$ , mostly in the range of  $10^3$ - $10^4$ . The number of edges is generally 1-10 times the corresponding node magnitude, ranging from  $10^3$ to  $10^6$ , with a majority falling in the range of  $10^3$ - $10^4$ . The features of citation network datasets are abundant ranging from  $10^3$  to  $10^5$  [53], [62], [87]. Graph classification tasks are typically applied in social network domains, with the number of graphs ranging from  $10^3$  to  $10^4$ , nodes around  $10^2$ ,

and edges around  $10^2$  [39], [57], [104]. These datasets often reflect connections between similar papers or users sharing common interests, displaying homogeneous graph structures. The size of bioinformatics networks is typically around  $10^2$ , with nodes and edges around  $10^1$ . While the number of features is less abundant compared to other domains [39], [57].

Molecular graphs represent atomic structures where nodes represent atoms, and edges represent chemical bonds. These datasets can serve as downstream datasets for evaluating the pre-training methods on the molecular property prediction task (a graph-level task). They are widely used for evaluating the transferability of pre-training methods and assessing the ability of pre-training methods to generalize across different distributions. The number of molecules ranges from  $10^3$  to  $10^4$ , with an average of around  $10^2$  nodes, and the number of prediction binary prediction tasks varies from 1 to  $10^2$  [57], [58]. Detailed information is listed in Table 3.

# 6.2.2 Heterogeneous Datasets

Compared to homogeneous datasets, heterogeneous datasets are relatively scarce. This scarcity is attributed to the limited number of research papers on heterogeneous graph prompt learning. We categorized heterogeneous datasets into three types: WebKB Webpage, Author Co-occurrence, and Wikipedia webpage. In the type of WebKB Webpage, nodes represent webpages from different computer science departments of different universities, and edges represent mutual links between webpages. The number of nodes and edges is around  $10^2$ , with features in the order of  $10^3$ . The number of nodes in other datasets is around  $10^3$ , with the edges around  $10^4$ , and features around  $10^3$  [62], [105]. Detailed information is provided in Table 4.

# 7 UNDISOLVED PROBLEM AND FUTURE WORK

In this section, we summarize the unsolved problems of current research works. Furthermore, we discuss the future research directions to pave the way for advancements in this promising area.

TABLE 3: Detailed summarization of protein and molecular datasets.

Dataset	#. Proteins / Molecules	Avg. # Nodes	# Tasks	Source
PPI	88k	-	40	
BBBP	2039	24.1	1	
Tox21	7831	18.6	12	
ToxCast	8575/8576	18.8	617	
SIDER	1427	33.6	27	GPF [64], SGL-PT1 [57]
ClinTox	1478/1477	26.2	2	
MUV	93087	24.2	17	
HIV	41127	24.5	1	
BACE	1513	34.1	1	

TABLE 4: Detailed summarization of heterogeneous graph datasets.

Type	Dataset	Hnode	Hedges	#. Avg. Nodes	#. Avg.Edges	#.Feature	#. Classes	Source
WebKB Webpage	Cornell Texas Wisconsin	0.11 0.06 0.16	0.30 0.11 0.21	183 183 251	295 309 499	1,703 1,703 1,703	5 5 5	PGCL [62], heter-graphs [105] PGCL [62], heter-graphs [105] PGCL [62], heter-graphs [105]
Author Co-occurrence	Actor	0.24	0.22	7,600	33,544	931	5	heter-graphs [105]
Wikipedia Webpage	Chameleon Squirrel	0.25 0.22	0.23 0.22	2,277 5,201	36,101 217,073	2.325 2,089	5 5	PGCL [62], heter-graphs [105] heter-graphs [105]

#### 7.1 Undisolved Problem

Despite the demonstrated efficacy of graph prompts in a variety of graph-related tasks, current methodologies are predominantly empirically driven, with limited theoretical underpinning. In this section, we delineate the principal limitations of graph prompts, categorized into the following four main issues.

Theoretical Foundations. Existing graph prompt methods often extrapolate ideas from natural language processing (NLP) and computer vision (CV) prompts or extend properties from graph pre-training paradigms. However, there is a notable lack of comprehensive theoretical analysis elucidating why prompts facilitate the seamless transfer of pre-training knowledge. The theoretical basis for the effectiveness of graph prompts remains largely unexplored.

Robustness. While it is hypothesized that graph prompts may be more robust than the fine-tuning paradigm, current methodologies lack empirical validation. Several critical aspects warrant further investigation. Firstly, the resilience of graph prompt methods to adversarial attacks has not been adequately studied. Secondly, the stability of graph prompt methods during the optimization process remains under-examined. Finally, a rigorous evaluation of the overall robustness of graph prompt methods compared to traditional approaches across diverse scenarios is needed to ensure their practical applicability and reliability.

Datasets and Evaluation Criteria. Several challenges exist in the description and establishment of datasets and evaluation criteria. Initially, discrepancies in the reported values of the same properties for the same dataset across multiple papers were identified, including differences in the numbers of nodes, edges, and features. These discrepancies may stem from inconsistencies in the evaluation and definition of properties or different feature selection criteria. Additionally, the lack of a unified standard for describing experimental processes and introducing datasets leads to unclear and incomplete descriptions. Ultimately, the diversity and scattered nature of datasets result in the absence of

canonical datasets applicable to graph prompt learning.

Universal Applicability. Graph prompts are less universally applicable in graph learning compared to their well-established counterparts in NLP with large language models (LLMs). Unlike LLMs, where prompts can guide text generation across various topics due to the consistent structure of language, graph prompts must be tailored to the specific characteristics of individual graphs and tasks. This necessity arises from the significant variability in graph structures and attributes, challenging the development of a unified prompting mechanism. While specialized graph prompts enhance performance through domain-specific knowledge, they detract from the goal of creating a generalized model capable of handling diverse graph-based tasks with a single unified approach.

## 7.2 Future Research Directions

Addressing the aforementioned limitations will contribute significantly to advancing the field of graph prompt learning. Future research should focus on the following directions:

Establishing Theoretical Foundations. Future research should aim to establish a robust theoretical framework to comprehend the mechanisms underpinning the efficacy of graph prompts in the graph domain. This includes a comprehensive theoretical analysis elucidating why prompts facilitate the seamless transfer of pre-training knowledge.

Enhancing Robustness. Research should investigate the resilience of graph prompt methods to adversarial attacks, evaluate their stability during the optimization process, and conduct rigorous evaluations of their overall robustness compared to traditional approaches across diverse scenarios. Understanding these aspects will lead to the development of more stable and reliable graph prompt methods.

Standardizing Datasets and Evaluation Criteria. Establishing standardized datasets and evaluation criteria is essential for advancing the field, especially for large-scale datasets such as the OGB benchmark [26]. This includes resolving discrepancies in reported values of dataset properties,

unifying standards for describing experimental processes and datasets, and creating canonical datasets applicable to graph prompt learning.

Achieving Universal Applicability. Efforts should be directed toward developing a more generalized model capable of handling diverse graph-based tasks with a single unified approach. This involves addressing the significant variability in graph structures and attributes and creating prompts that can be universally applicable across different graph learning tasks.

Improving Expressiveness. Future studies should explore how graph prompts can amplify the expressiveness of GNNs and whether they can transcend the inherent limitations of traditional GNNs. Systematic investigation into the potential enhancement of expressiveness through graph prompts is necessary.

# 8 Conclusion

This survey delves into the promising intersection between AGI and graph data through the lens of graph prompt learning. Our unified framework provides a structured understanding of graph prompts, categorizing them into tokens, token structures, and insertion patterns. This novel contribution offers clarity and comprehensiveness for both researchers and practitioners. By examining the interplay between graph prompts and models, our survey unveils new insights into the fundamental framework of graph prompt learning. We highlight their pivotal role in reshaping AI applications for graph data, demonstrating their potential to enhance model performance, adaptability, and efficiency. Furthermore, our survey outlines a clear roadmap for the future of graph prompt learning. We discuss the existing challenges, such as the diverse nature of graph-structured data and the gaps between the pre-training and downstream fine-tuning phases. The comprehensive discussions and analyses provided in this survey serve as a beacon for the evolving field of graph prompting. By identifying and addressing the current limitations, we pave the way for advancements that will further bridge the gap between AGI and practical applications involving graph data. Our survey underscores the transformative potential of graph prompt learning, emphasizing its significance for future research and applications.

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