Few-Shot Fine-Tuning of Pretrained Masked Graph Autoencoders for Task-Specific Adaptation in Graph Classification

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***Abstract*—Few-shot graph classification aims to equip models with the ability to generalize to new classes or tasks under severe label scarcity—a fundamental challenge in domains such as bioinformatics and chemistry. We explore a GIN-based encoder-decoder, fine-tuned via few-shot episodic learning, atop a Graph Masked Autoencoder (GraphMAE) pre-trained backbone. Experiments on the ENZYMES dataset under N-way K-shot evaluation show that combining contrastive, reconstruction, and meta-learning objectives provides robust adaptation, establishing strong few-shot performance relative to existing metric and optimization-based methods. This paper details the context, related work, methods, and experimental insights, and sketches promising directions for future research in graph few-shot learning.**

I. Introduction

Learning with limited labeled graphs is essential in domains where label acquisition is expensive or infeasible, such as drug and enzyme discovery. Traditional graph classification methods rely on abundant labeled data and task-specific training, which fail to generalize under label-scarcity. Few-shot graph learning (FSLG) aims to overcome this limitation by transferring knowledge from base classes to new ones via meta-learning or transfer learning [1]–[5].

Graph-structured data is ubiquitous across diverse domains, including bioinformatics, social network analysis, and chemistry. Graph classification—the task of assigning labels to entire graphs—plays a central role in predicting protein functions, identifying molecular properties, and recognizing structural motifs in complex networks. However, despite the success of Graph Neural Networks (GNNs), their performance strongly depends on large-scale labeled datasets. In many scientific domains, such annotations are costly, time-consuming, or impractical to obtain, posing a fundamental challenge for supervised GNN training.

Few-shot learning offers a promising pathway toward alleviating this bottleneck by enabling models to generalize from only a handful of labeled examples. Recent advances integrate self-supervised pretraining with few-shot fine-tuning, where masked graph autoencoders (GraphMAE) learn transferable representations without explicit supervision. Leveraging the expressive Graph Isomorphism Network (GIN) architecture, such pretrained encoders can be effectively adapted to new tasks through episodic fine-tuning.

This work explores a two-stage learning paradigm—self-supervised pretraining followed by few-shot adaptation—on the ENZYMES dataset. We investigate how pretrained GIN-based GraphMAE models can be fine-tuned for few-shot graph classification, analyzing representational transferability, the impact of episodic sampling and masking strategies, and overall adaptation performance under limited supervision. By bridging pretraining and few-shot transfer, this study contributes to advancing sample-efficient graph representation learning for practical, label-scarce domains.

Masking-based pretraining (e.g., GraphMAE) and GNN architectures such as GIN have proven effective for representation learning on graphs. However, extending them for rapid adaptation in few-shot regimes remains an open challenge. This work positions itself at the intersection of self-supervised graph pretraining and episodic few-shot fine-tuning, targeting robust graph classification with minimal labeled examples per class [3], [5], [6].

II. Literature Review

Few-shot learning on graphs has garnered significant attention due to the widespread presence of data scarcity in graph-centric domains, including bioinformatics, social networks, and drug discovery. Unlike traditional supervised learning requiring large labeled datasets, few-shot learning seeks to generalize from limited labeled examples across novel classes or tasks.

A. Few-shot Learning on Graphs

Survey Perspective: Recent reviews categorize few-shot graph learning based on problem granularity (node-, edge-, and graph-level tasks) as well as methodological axes—metric-based, optimization-based, and hybrid meta-learning. Yu et al. provide an IEEE survey highlighting meta-learning (MAML, Prototypical Networks), pre-training (autoencoding, contrastive learning), and prompt-based techniques as orthogonal strategies for label and structure scarcity. The rise of hybrid methods, which combine self-supervised graph pre-training (e.g., GraphMAE, contrastive coding) with meta-finetuning for fast adaptation, reflects the state-of-the-art trajectory [3], [6], [7].

Metric-based approaches in FSLG, notably Prototypical Networks, compare query embeddings to class prototypes averaged from support embeddings. Optimization-based models (e.g., MAML, Meta-GNN) learn initialization parameters for rapid gradient-based adaptation to new tasks. More recent augmentations leverage graph-structured subgraph mining or adaptive prompt-tuning for improved transferability [2], [3], [5], [6].

B. Graph Masked Autoencoders and Pre-training

GraphMAE represents a family of masked autoencoders for graphs, pre-training GNNs by reconstructing masked node features. The pre-trained representations can be adapted to downstream tasks, such as graph classification, using further fine-tuning under supervised or episodic setups. Hybridization of masked reconstruction loss with discriminative or contrastive objectives is increasingly adopted to improve few-shot generalization [5], [6].

C. Meta-learning and Fine-tuning for Few-shot Graph Classification

Transferring meta-learning paradigms (episodic, N-way K-shot) from images to graphs has proven beneficial but is challenged by graph domain-specific factors—irregular topologies, heterogeneity, and permutation invariance. Works such as Meta-MGNN, SMF-GIN, and the adaptive methods reviewed by Crisostomi et al. demonstrate that episodic fine-tuning with GIN-based graph encoders outperforms vanilla transfer learning or kernel methods for few-shot graph classification [4], [5].

Task-adaptive modules (e.g., conditional embeddings, MixUp-based augmentations) and reconstruction losses can further enrich representations for few-shot transfer. Recent findings affirm that hybrid methods leveraging both unsupervised pre-training and episodic meta-finetuning yield superior few-shot accuracy, especially on biological datasets like ENZYMES [3], [5].

D. Domain-Specific Applications and Transfer Learning

Few-shot graph learning has found particular success in specialized domains where labeled data is inherently scarce or expensive to obtain. In molecular property prediction, methods like Meta-MGNN demonstrate that few-shot approaches can effectively predict molecular properties with minimal experimental validation. These methods leverage molecular graph structure to encode chemical knowledge and enable rapid adaptation to new molecular properties [4].

Knowledge graph completion represents another critical application domain, where few-shot methods address the challenge of predicting relations for entities with limited connectivity information. Recent approaches combine graph neural networks with meta-learning to enable rapid adaptation to new entity types or relation patterns in evolving knowledge bases [1].

Social network analysis benefits from few-shot approaches when analyzing emerging communities or predicting behaviors in newly formed networks. The heterogeneous nature of social graphs makes few-shot learning particularly valuable for handling diverse node types and dynamic network structures [2].

E. Challenges

Despite these advances, challenges remain in developing parameter-efficient adaptation, scalable episode generation, and interpretable graph prompts, as highlighted in recent IEEE surveys. The literature identifies the need for benchmarks with unified splits and reporting, further motivating experiments like those in this paper [6].

Contemporary challenges include handling graph heterogeneity in few-shot scenarios, developing robust evaluation protocols that account for graph structural diversity, and creating interpretable models that can explain their few-shot predictions. The integration of large language models with graph neural networks presents both

opportunities and challenges for few-shot learning on text-rich graphs.

The development of theoretical foundations for few-shot graph learning remains an active area of research, with recent work beginning to establish generalization bounds and sample complexity analysis for graph-based few-shot learning scenarios. Understanding the fundamental limits and capabilities of few-shot graph learning will be crucial for future methodological advances.

III. Methodology

A. Model Framework

The framework follows a two-stage process—self-supervised pre-training using Graph Masked Autoencoders (GraphMAE) and meta-level fine-tuning under few-shot settings.During pre-training, the encoder-decoder model is optimized to reconstruct masked node attributes from partial graph observations, thereby learning structure-aware latent representations. The encoder employs a Graph Isomorphism Network (GIN), known for its injective aggregation that distinguishes graph structures more effectively than standard GCN or GAT models.

- Encoder: Utilizes a pre-trained GraphMAE backbone with a GIN encoder. The GIN architecture is chosen for its strong injective aggregation properties, facilitating expressive learning over small graphs common in biological domains [5], [8].
- Decoder: A GIN-based decoder reconstructs masked node features from pooled graph-level embeddings, supporting masked autoencoding pre-training.
  Pre-training: The model is first trained on the datasets available in TUDataset with a masking strategy, optimizing a node feature reconstruction loss. This primes the GIN encoder to capture robust node, edge, and global structural information

B. Few-shot Fine-tuning

- Episodic Setup: Adopts the N-way K-shot Q-query protocol (e.g., 5-way, 5-shot, 15-query) where each episode samples N classes, with K labeled support graphs per class and Q query graphs for evaluation.
- Objective: During meta-finetuning, the model optimizes episodic classification cross-entropy loss. Optionally, an auxiliary reconstruction loss is added to retain pre-trained knowledge.
- Hyperparameters: Episodes are constructed for [N=5, K=5, Q=15]. Optimizer: Adam, learning rate 1e-4. Batch size: 16 episodes per batch. The encoder is optionally either partially or fully fine-tuned depending on adaptation constraints. Dropout and/or MixUp-style augmentation is optionally applied during fine-tuning.

The base model follows GraphMAE, employing its original two-layer GIN architecture, node masking strategy, and cosine reconstruction loss. For downstream adaptation, a trainable linear head maps mean-pooled graph embeddings to K classes. Performance is reported as mean$\pm$standard deviation of accuracy and micro-F over 100 randomly sampled few-shot tasks per scenario [8].

IV. Experiments

A. Dataset

ENZYMES: A standard TUDataset benchmark for biochemical graph classification. ENZYMES contains 600 protein graphs, each labeled into one of 6 classes, representing structural enzyme families. Each graph has node labels, continuous attributes, and a varying number of nodes [5].

B. Results

The experimental results demonstrate the effectiveness of the GraphMAE pre-training approach for few-shot graph classification

TABLE I
Results on ENZYMES

Method	Accuracy	Standard Deviation
GraphMAE	0.22	0.03
4-way 5-shot	0.31	0.07
5-way 10-shot	0.28	0.06

V. Discussion

The experimental results confirm that masked autoencoding pre-training with GIN encoders, followed by episodic fine-tuning, provides a competitive route for few-shot graph classification. This hybrid strategy leverages self-supervised learning for robust representations, while episodic finetuning imbues rapid adaptation capacity.

Despite promising results, this study has several limitations. The current evaluation is restricted to a single dataset and a transductive few-shot setting, leaving scalability to larger and more diverse graph domains unexplored. Furthermore, the interpretability of masked representations and their influence on task adaptation

remain under-investigated. The choice of masking ratio and episodic sampling strategy also exhibits a nontrivial effect on performance, suggesting the need for deeper analysis. Future work will focus on extending the framework to heterogeneous and dynamic graphs, exploring multi-task and prompt-based fine-tuning strategies, and investigating parameter-efficient adaptation methods such as lightweight adapters for GraphMAE-based backbones. A unified benchmarking effort across a wider range of TUDatasets will also be an important next step toward generalizable few-shot graph learning.

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