Pre-train Graph Neural Networks for Brain Network Analysis (Extended Abstract)

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***Abstract*—Human brains, controlling behaviors and cognition, are at the center of complex neurobiological systems. Recent studies in neuroscience and neuroimaging analysis have reached a consensus that interactions among brain regions of interest (ROIs) are driving factors for neural development and disorders. Graph neural networks (GNNs) as a powerful tool for analyzing graph-structured data are naturally applied to the analysis of brain networks. However, training of deep learning models including GNNs often requires a significant amount of labeled data. Due to the complicated data acquisition process and restrictions on data sharing, brain network datasets are still small compared to other types of graphs (e.g., social networks, molecules, proteins). Moreover, real clinical tasks (e.g., mental disorder analysis) are often conducted on local datasets with even smaller scales and larger noises. To this end, we propose to leverage pre-training to capture the intrinsic brain network structures regardless of specific clinical outcomes, for obtaining GNN models that are easily adaptable to downstream tasks. Specifically, (1) we design brain-network-oriented unsupervised pre-training techniques to utilize large-scale brain imaging studies without highly relevant task labels; (2) we develop a data-driven parcellation atlas mapping pipeline to facilitate effective knowledge transfer across studies with different ROI systems. The proposed framework is validated with various GNN models, with extensive empirical results demonstrating consistent improvement in performance as well as robustness.**

***Index Terms*—Brain Network Analysis, Pre-training, GNN**

I. Introduction

In recent years, the analysis of brain networks has attracted considerable interest in neuroscience studies. Brain networks are essentially graphs, where anatomical regions of interest (ROIs) given a parcellation atlas are formed into nodes, and the connectivities among ROIs are formed into edges. Based on brain networks constructed from different modalities such as Diffusion Tensor Imaging (DTI) and functional Magnetic Resonance Imaging (fMRI), effective graph analysis plays a pivotal role in understanding the biological structures and functions of complex neural systems, which can be helpful in the early diagnosis of neurological disorders and facilitate neuroscience research [1].

Deep learning has replenished the fields of computer science and beyond. Among various modern deep learning models, the emerging graph neural networks (GNNs) have demonstrated superior performance and even plausible interpretability on a variety of network datasets, including social networks, recommender systems, knowledge graphs, protein and gene networks, molecules, and so forth [2], [3], due to its powerful representations and efficient computations of complex graph structures towards specific downstream tasks. Such achievements on other types of networked data propel studies on GNNs for brain networks, especially models for graph-level classification/regression [3] and important vertex/edge identification [4], towards tasks such as connectome-based disease prediction and multi-level neural pattern discovery. However, training powerful deep learning models including GNNs often requires significant amounts of labeled data [5]. For brain network analysis, there are limited big imaging datasets from a few large-scale national neuroimaging studies such as the ABCD [1], ADNI [2], and PPMI [3]. However, such datasets are still rather small compared to graph datasets in other domains (e.g., datasets with 41K to 452K graphs on OGB [4] and datasets with thousands to millions of graphs on NetRepo [5]).

One solution toward data scarcity is transfer learning which transfers models trained on large-scale brain network datasets onto small-scale local studies while retaining favorable performance. However, one limitation of transfer learning is its reliance on the availability of similar tasks as supervision during training in the source dataset. In reality, similar tasks in the smaller local studies may not always be available in the large-scale public studies. Pre-training has shown its effectiveness in the fields of computer vision [6], natural language processing [7], as well as graph mining [8]. We explore GNN pre-training on brain networks without supervision and study its effectiveness in predicting specific clinical outcomes. However, unique challenges impede the direct application of existing GNN pre-training paradigms to brain networks. For example, brain networks within one study usually share the same node system, which is not properly exploited, whereas different studies often use different node systems, which hinders the transferability of pre-trained models.

[1] https://abcdstudy.org/study-sites/
[2] https://adni.loni.usc.edu/
[3] https://www.ppmi-info.org/
[4] https://ogb.stanford.edu/
[5] https://networkrepository.com/

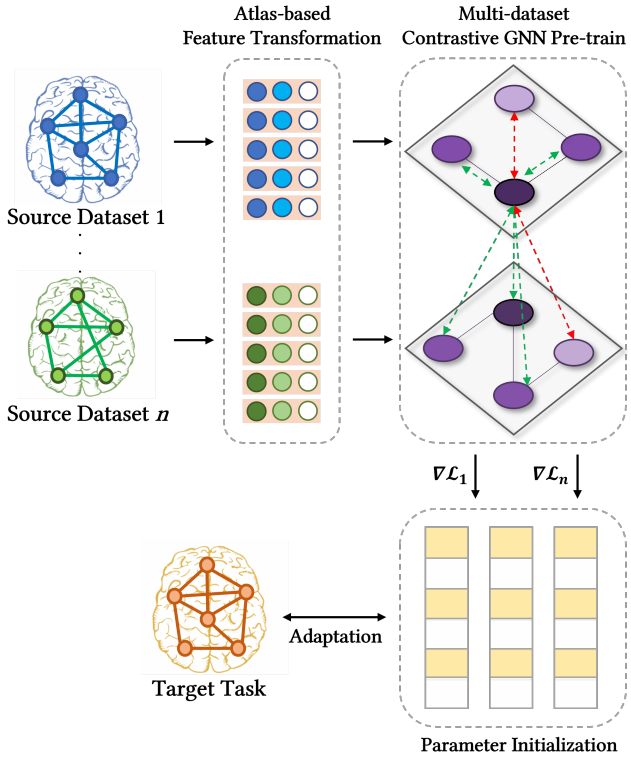

Fig. 1. Overview of our proposed framework. We first project the source data features into a fixed dimensional representation through atlas transformation. We then pre-train a GNN encoder under the proposed multi-dataset contrastive learning. Finally, learned parameters are fine-tuned on a target task.

In this work, we first formulate our problem into a self-supervised multi-dataset GNN pre-training objective. Specifically, our goal of model pre-training is to obtain a general parameter initialization that contains relevant knowledge of brain network characteristics and can achieve efficient downstream adaptation on target datasets typically of smaller scales. To this end, we adapt the popular data-efficient framework of MAML [9] as our base pre-training architecture which advantageously allows fast optimization of GNN models on multiple data domains. Moreover, we illustrate a high-level overview of our proposed pipeline workflow in Figure 1.

As the second and most important contribution, we leverage the graph contrastive learning paradigm to shape a unified pre-training objective and propose a novel brain-network-oriented contrastive sampling strategy. In particular, since brain networks within one dataset are defined by a fixed node system that shares identical node orderings, we can promote GNN to learn on shared substructure knowledge. Hence, we can naturally extend to a multi-graph intra-dataset setting when we are constructing the contrastive samples with respect to given anchors. In addition, to facilitate an intuitive understanding of our unique sampling considerations, we propose to categorize the possible sample selections into four different types. Furthermore, our categorization can also be adapted to describe the objective formulations in various state-of-the-art graph-based contrastive learning frameworks [10]–[14].

As the third contribution, different brain network datasets are parcellated under different atlas systems, which leads to varying dimensionalities and semantics of initial features, and such misalignment can negatively affect downstream adaptation. To this end, we develop a data-driven pre-processing solution through linear autoencoders that project original features into a lower dimensional space shared across all datasets. To have the transformed features maximally preserve the original structural information, our solution also presents three carefully chosen regularizers to guide the optimizations of the autoencoders. In addition, we also propose to apply variance-based sorting to the projected features to achieve cross-dataset alignment.

We conduct extensive experiments to evaluate the proposed pipeline on downstream disease classification objectives. Compared to a spectrum of chosen baselines adapted to our setting, our framework reflects superior results across all metrics including accuracy scores and area under the ROC curve. We further the empirical analysis through in-depth ablation studies and our findings validate the positive contributions to the overall performance of each constituent component of our framework. Besides, we also evaluate the pre-training and fine-tuning efficiency of GNN models optimized under our framework through visual comparisons, and our fully-loaded framework demonstrates the fastest and most robust source convergence as well as target adaptation.

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