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# Self-supervised Learning with Adaptive Graph Structure and Function Representation For Cross-Dataset Brain Disorder Diagnosis

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**Abstract.** Resting-state functional magnetic resonance imaging (rs-fMRI) helps characterize the regional neural activity of the human brain. Currently, supervised deep learning methods that rely on a large amount of fMRI data have shown good performance in diagnosing specific brain diseases. However, there are significant differences in the structure and function of brain connectivity networks among patients with different brain diseases. This makes it difficult for the model to achieve satisfactory diagnostic performance when facing new diseases with limited data, thus severely hindering their application in clinical practice. In this work, we propose a self-supervised learning framework based on graph contrastive learning for cross-dataset brain disorder diagnosis. Specifically, we develop a graph structure learner that adaptively characterizes general brain connectivity networks for various brain disorders. We further develop a multi-state brain network encoder that can effectively enhance the representation of brain networks with functional information related to different brain diseases. We finally evaluate our model on different brain disorders and demonstrate advantages compared to other state-of-the-art methods.

**Keywords:** Resting-state fMRI · Brain Connectivity Network · Graph Contrastive Learning · Graph Structure Learning

## 1 Introduction

Resting-state functional magnetic resonance imaging (rs-fMRI), as a non-invasive tool, has demonstrated its potential to evaluate brain activity by measuring blood oxygen level-dependent (BOLD) signals over time [23,25]. Despite existing deep learning methods have made progress in the analysis of brain networks

based on fMRI, they are mainly targeted at specific brain diseases and struggle to be generalized to unseen diseases with satisfactory diagnosis performance [4,11,15]. Generally, different diseases can cause distinct brain functional impairments, leading to variations in the distribution of brain connectivity network structure and function among individuals. Therefore, when faced with new brain diseases, it is typically needed to train a new diagnostic model using an extensive collection of data, which poses significant challenges for clinical practice, particularly in the diagnosis of rare diseases.

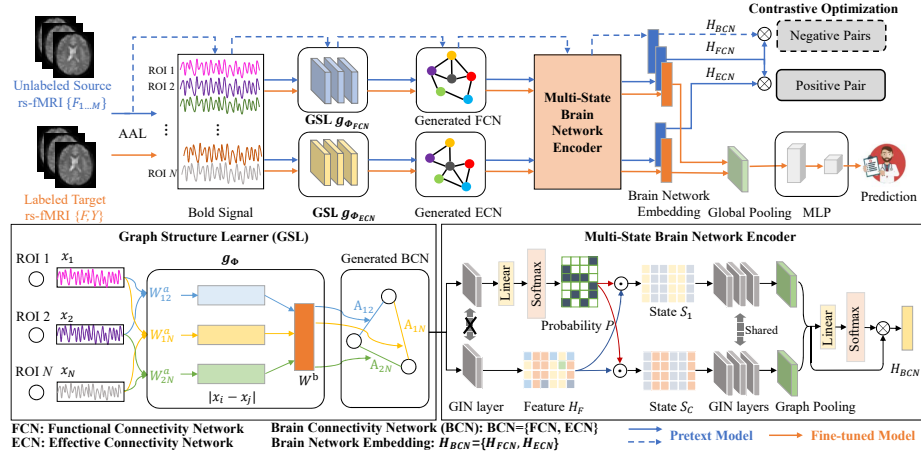
Recently, self-supervised learning (SSL) has emerged as a promising learning paradigm that can extract information from the underlying structure and features of limited data without specific task constraints [12,14]. Among them, contrastive-based methods extract effective representations by learning to discriminate positive and negative instance pairs, which have been proven to have exceptional generalization capabilities [10,22]. However, there remain two challenges: **1) How to construct optimal paired instances that can model generalizable knowledge from various brain disorders?** Previous studies mainly focused on the design of brain connectivity networks (BCNs) in different scales. For example, Wang [22] utilized two time windows to construct two functional connectivity networks (FCN) respectively. Yang [27] defined several subgraphs based on the brain sub-network pattern. However, all of these brain networks are pre-defined and remain fixed, making it hard to obtain generalized information among various brain disorders. **2) How do we fully explore the characteristic information of brain networks to obtain the optimal representation for downstream disorder diagnosis tasks?** Studies on brain functional dynamics have shown that the brain network contains a variety of functions during activities, and different functional impairments may lead to various brain diseases [1,29]. However, existing methods have few concerns about this functional heterogeneity, which may lead to suboptimal representations.

To address the aforementioned issues, we propose a novel self-supervised graph contrastive learning method (illustrated in Fig. 1). The main contributions of this paper are as follows: 1) We develop a novel framework for cross-dataset brain disorder diagnosis, which allows to perform self-supervised pre-training of brain networks and transfer them to unseen brain diseases, addressing the problem of resource-limited training. 2) We propose a novel graph structure learner that can adaptively generate different views of brain connectivity networks and capture general structural information for various brain disorders. 3) We construct a multi-state brain network encoder to capture distinct brain functional information, enabling the extraction of adaptive brain network representations tailored to different brain disorders.

## 2 Method

### 2.1 Preliminary

**Problem Formulation.** We define the cross-dataset brain disorder diagnosis task using input datasets with  $D = \{D_{source}, D_{target}\}$ , where  $D_{source} = \{F_i\}_{i=1}^M$ ,



**Fig. 1.** Overview of our proposed framework, which includes a pretext model (i.e., blue line, where the solid and dash lines represent positive and negative instances respectively) and a fine-tuned model (i.e., orange line). The pretext model consists of two core modules: 1) a graph structure learner generating two different brain connectivity networks (i.e., FCN and ECN) from the bold signal; 2) a multi-state brain network encoder that encodes brain networks into multiple brain states and learns a comprehensive representation. Fine-tuned model initializes with pretext parameters and fine-tunes using labeled target fMRI data.

and  $D_{target} = \{F_i, Y_i\}_{i=1}^L$ . Here,  $F$  is the fMRI data, and  $Y$  is the label set of all target subjects. ROIs are defined in individual fMRI spaces based on the AAL atlas [20] to extract ROI-based fMRI signals  $X = (x_1, x_2 \dots x_N) \in \mathbb{R}^{N \times T}$ , where  $N$  is the number of ROIs and  $T$  is the time points for bold signals. The pretext model is pre-trained using the  $D_{source}$  dataset and then fine-tuned on a randomly selected subset of labeled data from the target dataset. The model finally predicts results  $\hat{Y}$  for the remaining test subjects in the target dataset.

**Brain Connectivity Network.** Brain connectivity networks are typically categorized as either functional connectivity networks (FCN) or effective connectivity networks (ECN) based on different interrelated aspects of brain organization [9]. FCN describes brain activity from the perspective of statistical dependencies between brain regions, which is usually estimated by correlation measures [17]. In contrast, ECN refers to the directional effects that one brain region exerts over another, which can be inferred through time series causality measurements such as transfer entropy [18].

**Functional Brain State.** The brain network relies on coordinating various functions during the activity process, which exhibits distinct functional configurations, also known as "brain states" [19,3]. These different brain states depict the diverse functional characteristics of the brain network, which can be characterized by discriminating features constructed from brain connectivity networks.

## 2.2 Pretext Model

**Graph Structure Learner.** To establish a contrastive framework based on paired instances, we initially construct two distinct brain connectivity networks for each subject. The conventional method involves utilizing a pre-defined graph such as FCN or ECN. However, these graphs are generally sensitive to local noise and exhibit significant distribution variance across different subjects of brain disorders. Therefore, we directly generate brain connectivity networks from the bold signals and continuously optimize the graph structure through model training to ensure optimal connectivity.

Specifically, for each subject with a series of bold signals  $X = (x_1, x_2 \cdots x_N) \in \mathbb{R}^{N \times T}$ , our goal is to find a non-negative  $\Phi$  parameterized generation function  $A_{i,j} = g_{\Phi}(x_i, x_j)$  to construct a brain connectivity network, where each element represents the pairwise relationship between ROI  $i$  and ROI  $j$ . Considering that there are two different patterns of brain network connectivity, we design two implements  $g_{\Phi} = \{g_{\Phi_{FCN}}, g_{\Phi_{ECN}}\}$  according to different interaction characteristics of the connections. We first utilize Pearson correlation  $\rho(x_i, x_j)$  [2] and transfer entropy  $\zeta(x_i, x_j)$  [21] to measure the structural relationship  $W_{ij}^a$  between paired ROIs, respectively, which can be formulated as  $W_{ij}^a = \{\rho(x_i, x_j), \text{if } g_{\Phi} = g_{\Phi_{FCN}}; \zeta(x_i, x_j), \text{if } g_{\Phi} = g_{\Phi_{ECN}}\}$ . Considering the optimization of graph structure, we continue to measure the attention relationship via a learnable weight vector  $W^b = (w_1, w_2, \dots, w_T)^T \in \mathbb{R}^{T \times 1}$  and an absolute difference operation between the paired ROIs. Finally, we integrate structural information with attention relationships to generate a brain connectivity network as

$$A_{ij} = g_{\Phi}(x_i, x_j) = \frac{W_{ij}^a \exp\left(\text{ReLU}\left(W^{bT} |x_i - x_j|\right)\right)}{\sum_{j=1}^n W_{ij}^a \exp\left(\text{ReLU}\left(W^{bT} |x_i - x_j|\right)\right)}. \quad (1)$$

It is worth noting that, due to the bidirectional and unequal process of information transmission (i.e.,  $W_{ij}^a = W_{ji}^a$ , if  $g_{\Phi} = g_{\Phi_{FCN}}$ , and  $W_{ij}^a \neq W_{ji}^a$ , if  $g_{\Phi} = g_{\Phi_{ECN}}$ ), the generated ECN based on the transfer entropy is represented as an asymmetric matrix, whereas the generated FCN based on the Pearson correlation calculation with exchangeability is represented as a symmetric matrix, which is different from each other.

**Multi-State Brain Network Encoder.** Considering the complex function features of brain networks induced by distinct brain states, we propose to build a multi-state brain network encoder to capture a comprehensive brain network representation that contains underlying functional information related to brain disorders.

Specifically, for each generated brain connectivity network (i.e., FCN or ECN), we first utilize two independent Graph Isomorphism Network (GIN) layers [26] to generate two embedding matrices, one for feature representation  $H_F = \text{GIN}_f(A, H; \theta_f)$  and one for probability embedding matrix  $H_P = \text{GIN}_p(A, H; \theta_p)$ . Here, GIN is a commonly used graph neural network with a

hidden layer dimension denoted as  $D$ .  $A \in \mathbb{R}^{N \times N}$  is a generated brain connectivity network learned by the graph structure learner,  $H \in \mathbb{R}^{N \times T}$  is the node feature matrix measured by bold signals, and  $\theta$  is the learnable weight of GIN layers. To obtain the assignment probability of each dimension of functional features in distinct brain states, we calculate the probability matrix  $P \in \mathbb{R}^{D \times C}$  based on the clustering of the probability embedding matrix  $H_P \in \mathbb{R}^{N \times D}$ , which can be formulated as:

$$P = \text{softmax} \left( \text{Linear}_{N \times C} (H_P^T) \right), \quad (2)$$

where the softmax function is applied in a row-wise fashion, and  $C$  is the number of brain states. Based on the feature embedding  $H_F \in \mathbb{R}^{N \times D}$  and assignment probability matrix  $P$ , we can obtain the representation of each brain state through the product of feature and its corresponding assignment probability as:

$$S_c = H_F \odot R\{P_c\}^T, c \in \{1 \dots C\}, \quad (3)$$

where  $R$  is a repeat function that extends the probability vector  $P_c \in \mathbb{R}^{D \times 1}$  to the same dimension of the node embedding matrix,  $\odot$  denotes element-wise multiplication. After assigning the feature matrix to distinct brain states, we extract the graph embedding in each state  $H_c \in \mathbb{R}^{1 \times D}$  via multiple GIN layers and a graph pooling layer  $H_c = \frac{1}{N} \sum_{i=1}^N \text{GIN}_i(A, S_c, \theta_i)$ . Here, the GIN layers in different states share weights to reduce the complexity of the model.

Given the inconsistent impact of different brain states on brain activity, it is natural to expect diverse contributions from each brain state’s representation to the overall brain network representation. Thus, we propose a weighted attentional fusion method to obtain a comprehensive brain network embedding:

$$H_{BCN} = \sum_{c=1}^C a_c H_c, \quad (4)$$

$$\{a_1, \dots, a_c\} = \text{softmax} \left( \text{Linear}_{D \times 1} (\{H_1, \dots, H_c\}) \right), \quad (5)$$

where the brain network embedding  $H_{BCN} = \{H_{FCN}, H_{ECN}\}$  is determined by the type of generated brain connectivity network, and the weighted attention mechanism allows the model to decide which functional brain state should rely on for specific brain disorders more adaptively.

**Pre-training Strategy.** To pre-train the model, we define a polynomial loss function, which includes a contrastive loss  $\mathcal{L}_{CL}$ , a graph structural learning loss  $\mathcal{L}_{GL}$ , and an assignment probability loss  $\mathcal{L}_{AP}$ .

For contrastive loss, we follow the previous works and use the normalized temperature-scaled cross-entropy loss (NT-Xent)[28]. In practice, the two generated brain connectivity networks (i.e., FCN, ECN) from the same input are regarded as the positive pair. The other networks from the same data batch  $B$  are negative pairs, the temperature parameter as  $\tau$ , then we have

$$\mathcal{L}_{CL} = -\frac{1}{B} \sum_{i=1}^B \log \frac{\exp(H_{FCN_i} \cdot H_{ECN_i} / \tau)}{\sum_{k=1, k \neq i}^{2B} \exp(H_{FCN_i} \cdot H_{BCN_k} / \tau)}. \quad (6)$$

For the graph structure learner, we optimize the graph structure  $A$  by minimizing the following loss function

$$\mathcal{L}_{\text{GL}} = \sum_{i,j=1}^N \|x_i - x_j\|_2^2 A_{ij} + \gamma \|A\|_F^2, \quad (7)$$

where a larger distance between ROIs encourages a smaller value  $A_{ij}$ , and the second term is used to control the sparsity of learned brain connectivity networks.

For the multi-state brain network encoder, since each row of the probability matrix represents the probability of allocating the feature of this dimension to different brain states, it should generally be close to a one-hot vector, i.e., each dimension feature is assigned to each brain state. Therefore, we design an assignment probability loss to reduce the uncertainty of mapping distribution:

$$\mathcal{L}_{\text{AP}} = \frac{1}{D} \sum_{i=1}^D H(P_i), \quad (8)$$

where  $H$  denotes the entropy function, and  $P_i$  is the  $i$ -th row of the probability matrix  $P$ . Finally, the pretext model can be trained with the proposed polynomial loss function  $\mathcal{L} = \mathcal{L}_{\text{CL}} + \alpha \mathcal{L}_{\text{GL}} + \beta \mathcal{L}_{\text{AP}}$  in a self-supervised manner.

### 2.3 Fine-tuned Model

To transfer the pretext model trained on a large-scale fMRI data from the source domain to downstream classification tasks, we fine-tune the model on the target data for analysis. As shown in Fig 1, the fine-tuned model consists of all the modules in the pretext model along with a graph pooling layer (with a sum pooling layer) and a MLP layer (with two fully connected layers). During the fine-tuning process, we initialize the graph learning structure module and the graph encoder module with the parameters learned from the pretext model. Subsequently, we utilize the graph pooling layer to integrate brain network information from two distinct views and ultimately perform brain disease classification employing the MLP. In the fine-tuned model, we employ cross-entropy loss to replace the contrastive loss for supervised learning updates.

## 3 Experiments

### 3.1 Dataset and Experimental Settings

We perform a cross-dataset classification task to validate our model, where the model is pre-trained on one dataset and subsequently fine-tuned on an unseen dataset. Specifically, the model is pre-trained using the ADNI dataset [16] with 705 unlabeled fMRI data. Then, fine-tuning is executed on the ABIDE dataset [7], which includes 104 health controls and 78 ASDs, and on the ADHD dataset [6], consisting of 60 health controls and 53 ADHDs, respectively. During the fine-tuning stage, we employ 5-fold cross-validation and record the average and standard deviation of the test results.

**Table 1.** Classification results (%) in terms of “mean(standard deviation)” achieved by different methods in two cross-dataset brain disorder versus health control classification tasks. The proposed method shows statistically significant improvements (with  $p < 0.05$ ) over all compared methods.

Model	ADNI $\Rightarrow$ ABIDE				ADNI $\Rightarrow$ ADHD			
	ACC	SEN	SPE	AUC	ACC	SEN	SPE	AUC
BrainGB [8]	75.1(1.78)	74.2(2.07)	75.3(2.29)	76.5(2.06)	61.5(2.48)	69.4(1.24)	54.2(1.97)	59.0(1.87)
BrainGSL [24]	77.8(2.45)	75.8(2.21)	83.9(2.47)	79.4(2.33)	67.1(2.43)	75.9(2.04)	59.4(2.51)	67.6(2.15)
UCGL [22]	79.5(2.01)	74.1(1.79)	86.7(1.81)	81.6(1.95)	70.2(1.95)	75.2(1.78)	61.7(1.02)	68.1(1.54)
Ours (w/o pretext)	76.4(2.43)	72.6(2.80)	83.2(2.15)	77.2(2.37)	64.9(2.13)	73.2(2.44)	59.5(2.78)	65.9(1.92)
Ours	<b>81.6(2.19)</b>	<b>77.3(1.45)</b>	<b>89.6(1.34)</b>	<b>84.3(1.92)</b>	<b>72.2(1.75)</b>	<b>78.7(1.92)</b>	<b>67.1(2.03)</b>	<b>71.3(1.66)</b>

To ensure a fair comparison, all fMRI data are pre-processed in a standardized protocol and parcellated using AAL atlas into 90 ROIs. For all GNN-based methods, including the proposed multi-state brain network encoder, we utilize three graph neural network layers followed by a graph pooling layer. The optimization process employs the Adam optimizer with a learning rate of  $1e-4$ , a weight decay of  $1e-5$ , and 500 training epochs. We train our model with parameters: brain state  $C = 7$ , temperature parameter  $\tau = 0.5$ , trade-off parameters  $\alpha = 0.01$ , and both  $\lambda$  and  $\beta$  set to 0.001, respectively. For detailed experimental settings, readers are referred to the supplementary materials.

### 3.2 Results and Discussion

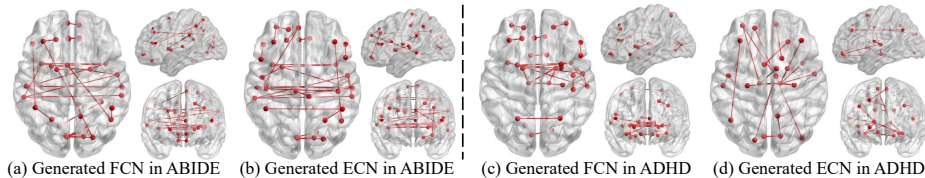
**Quantitative Analysis.** In Table 1, we compare our method with several SOTA methods [8,24,22]. It can be observed that: First, our method achieves superior performance than ours without pretext model, which proves that self-supervised methods can learn intrinsic brain information from large-scale brain network data and generalize it to new brain diseases. Second, when comparing two supervised methods (BrainGB vs. ours without pretext) that are directly applied to target datasets, it is evident that our method consistently achieves better performance, particularly in the ADHD dataset. This suggests that the specifically designed multi-state brain network encoder may exhibit more power than traditional graph neural networks in extracting efficient brain network representations for disorder diagnosis. Third, our method significantly outperforms other methods (including two self-supervised methods) in terms of all metrics. This improvement can be attributed to the utilization of augmented structural and functional information through distinct BCNs and a multi-state encoder, allowing for joint optimization of the general graph structure and representation during model training.

**Ablation Study.** We conduct ablation studies to verify the effectiveness of three key components: 1) the graph structure learner, 2) the multi-state brain network encoder, and 3) the polynomial loss function. In the graph structure learner, we compare our method with the traditional BCN construction method utilizing the same Pearson correlation and transfer entropy measurements. For the brain network encoder, we compare our multi-state method with a simple single-state encoder comprising 2 GIN layers and a graph pooling layer. In terms

**Table 2.** Ablation study of proposed method with different modules on cross-dataset classification tasks (%).

Model	Graph Structure		Encoder		Loss				Metrics			
	Learner	Fixed	Multi	Single	$\mathcal{L}_{GL}$		$\mathcal{L}_{AP}$		ADNI $\Rightarrow$ ABIDE		ADNI $\Rightarrow$ ADHD	
					w	o	w	o	ACC	AUC	ACC	AUC
1	✓		✓		✓		✓		75.8(3.25)	79.1(2.67)	69.5(2.31)	68.5(2.19)
2	✓		✓			✓	✓		53.2(3.58)	51.7(3.71)	51.0(2.97)	51.2(3.06)
3	✓			✓	✓			✓	75.1(2.34)	77.5(2.06)	65.5(1.93)	64.0(1.50)
4	✓			✓		✓		✓	52.6(2.98)	52.9(2.86)	52.1(2.71)	51.4(2.94)
5		✓	✓			✓	✓		77.5(2.31)	78.4(2.15)	69.7(1.88)	69.8(1.92)
6		✓		✓		✓		✓	75.9(1.54)	75.4(1.96)	62.3(1.94)	60.2(1.75)
7	✓		✓		✓		✓		<b>81.6(2.19)</b>	<b>84.3(1.92)</b>	<b>72.2(1.75)</b>	<b>71.3(1.66)</b>

of the loss function, we explore the impact of including graph structure learner loss and graph encoder loss. The classification results of all ablation studies are detailed in Table. 2. It can be observed that the proposed graph structure learner and multi-state brain network encoder are effective in two classification tasks (comparing models 3, 5, 6, and 7). In addition, the absence of the graph structure loss (in models 2 and 4) may make it difficult for the model to learn the valuable graph structure. Furthermore, the results of graph encoder loss ablation (comparing models 1, and 7) prove that the introduction of assignment constraint greatly enhances the robustness of the proposed model.

**Fig. 2.** Visualization of two brain connectivity networks generated by our method on ABIDE and ADHD datasets.

**Qualitative Analysis.** We visualize the top 30 most discriminative brain connections detected by our method in two datasets (Fig. 2). Comparing subfigures (a) and (b), as well as (c) and (d), we can find that two different types of BCNs can detect many overlapping brain connections that are consistent with the conclusion of [5,13], demonstrating the effectiveness of the graph structure learner in directing the model’s attention towards valuable connections. Moreover, several significant nodes that contain multiple connections are also identified as being associated with specific disorders (e.g., temporal detected by FCN and ECN in ABIDE, and amygdala in ADHD), which validates the effect of the proposed method for the diagnosis of different brain diseases.



## 4 Conclusion

In this paper, we present a novel self-supervised framework for analyzing brain connectivity networks and diagnosing cross-dataset brain disorders. Specifically, our model learns different brain connectivity networks and optimizes them through training to capture general patterns in various brains. We also develop a multi-state brain network encoder to capture the complex functional information associated with brain disorders. We demonstrate the superiority of our proposed model compared to other methods, and the ablation studies examine the effectiveness of each module in our proposed framework, as well as each item in the polynomial loss function. In the future, we plan to further expand the proposed method by incorporating inputs from multiple datasets and improve its applicability in real-world environments by using fewer fine-tuning target data.

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