Learnable Subdivision Graph Neural Network for Functional Brain Network Analysis and Interpretable Cognitive Disorder Diagnosis

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Abstract. Different functional configurations of the brain, also named as "brain states", reflect a continuous stream of brain cognitive activities. These distinct brain states can confer heterogeneous functions to brain networks. Recent studies have revealed that extracting information from functional brain networks is beneficial for neuroscience analysis and brain disorder diagnosis. Graph neural networks (GNNs) have been demonstrated to be superior in learning network representations. However, these GNN-based methods have few concerns about the heterogeneity of brain networks, especially the heterogeneous information of brain network functions induced by intrinsic brain states. To address this issue, we propose a learnable subdivision graph neural network (LSGNN) for brain network analysis. The core idea of LSGNN is to implement a learnable subdivision method to encode brain networks into multiple latent feature subspaces corresponding to functional configurations, and realize the feature extraction of brain networks in each subspace, respectively. Furthermore, considering the complex interactions among brain states, we also employ the self-attention mechanism to acquire a comprehensive brain network representation in a joint latent space. We conduct experiments on a publicly available dataset of cognitive disorders. The results affirm that our approach can achieve outstanding performance and also instill the interpretability of the brain network functions in the latent space. Our code is available at https://github.com/haijunkenan/LSGNN.

Keywords: Brain Network Analysis · Graph Neural Network · Brain States · Self-Attention Mechanism

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1 Introduction

Studies on brain functional dynamics show that the brain network contains a variety of distinct functional configurations (brain states) during the course of brain cognition activities [5,11]. These distinct brain states depict the heterogeneous functional signature of the brain network (e.g., Visual, Attention, etc.) [1]. Generally, brain states can be characterized by discriminate connections constructed from brain networks, and various strategies have been developed to identify brain states with the objective of understanding how heterogeneous information is represented in the brain [9,24]. For example, the whole-brain functional connectivity patterns derived from independent component analysis (ICA) are employed for brain network analysis [13,18]. However, they typically struggle to perform well on high-dimensional data and need further design techniques for feature selection.

Recently, graph neural networks (GNNs) have been proven to be helpful in brain network analysis, due to their powerful ability in analyzing graph-structured data [21]. However, the existing GNN methods for heterogeneity mostly deal with the semantic heterogeneity from different modalities [22,23] or the connectivity heterogeneity among nodes [10], and rarely consider the functional heterogeneity of the whole brain network. Therefore, it may lead to a suboptimal performance on disorder diagnosis. On the other hand, GNN as a deep learning model is typically poorly interpretable in brain network analysis [14]. Although several methods for GNN interpretation have been proposed, most of them concentrate on node-level or subject-level analysis. For instance, BrainGNN provides insights on the salient brain region of interest (ROIs) through specific node pooling operation [15]; IBGNN discusses the neural system mapping of subjects in different categories with an explanation generator mask [4]. However, few studies have been conducted on the interpretable analysis of brain states at network-level, especially the relationship between heterogeneous functional features of brain networks and corresponding disease diagnosis remains unexplored.

To address the above issues, we propose a learnable subdivision graph neural network to investigate brain networks with heterogeneous functional signatures, and the functional brain state can be combined with corresponding latent subspace for interpretable brain disorder diagnosis. The main contributions of this paper are as follows: 1)We propose a novel Learnable Subdivision Graph Neural Network (LSGNN) model for brain network analysis, which implements the extraction of heterogeneous features of brain networks under various functional configurations. 2) We develop a novel assignment method, that can encode brain networks into multiple latent feature subspaces in a learnable way. 3) Our method instills the interpretability of the latent space corresponding to brain states, which is beneficial to unveiling insights into the relationship between the signature of functional brain networks and cognitive disorder diagnosis.

2 Method

The framework of the LSGNN method is presented in Fig. 1, which is composed of three major components: the functional subdivision block (FSB), multiple GNN modules including the GNN layer (with shared weights) and graph pooling layer, and the functional aggregation block (FAB). Here, FSB is designed to automatically learn an assignment matrix to obtain the mask of each brain state. The inputs of FSB are acquired using two separate GNN layers with the same structure but different parameters. Furthermore, multiple GNN modules are designed to learn brain network representations under distinct brain states. Finally, FAB is developed to aggregate the information into a joint latent space, and acquire a comprehensive brain network representation for brain disorder diagnosis.

2.1 Preliminary

Problem Definition. The input of proposed model is a set of N weighted brain networks. For each network $\mathcal{G} = \{\mathcal{V}, \mathcal{E}, A\}$, $\mathcal{V} = \{v_i\}_{i=1}^{M}$ involves M nodes defined by the ROIs on a specific brain parcellation [7], and $\mathcal{E}$ records the distinct edge connections in each subject, which is represented with a weighted adjacency matrix $A \in \mathbb{R}^{M \times M}$ describing the correlation strengths among ROIs. The model finally outputs the prediction result $\hat{y}_n$ for each subject n.

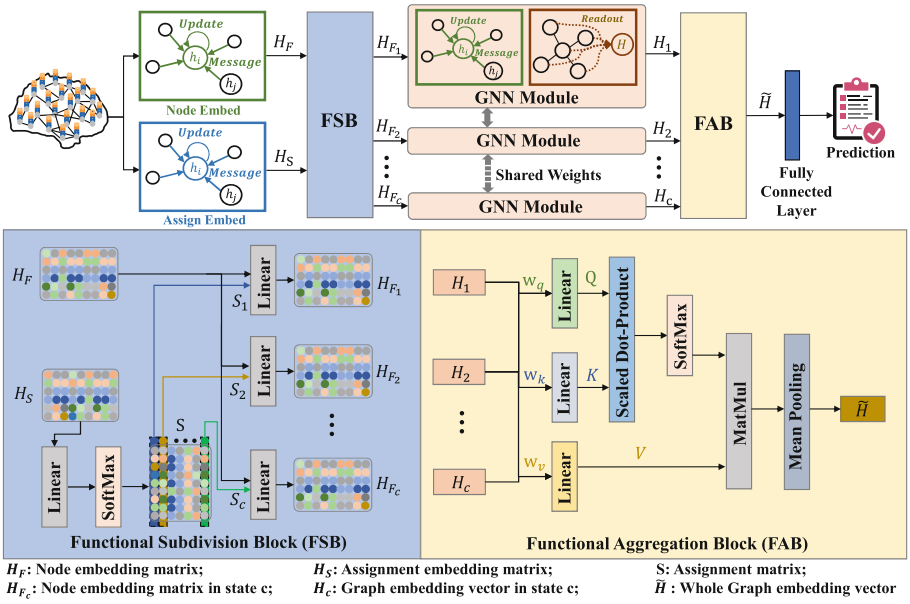

Fig. 1. Overview of the LSGNN framework which consists of FSB and FAB modules for learnable subdivision embedding and comprehensive brain network representation, respectively.

The GNN Module. The GNN module is superior in extracting structural information from the network, which is attributed by two kinds of layers [3]: 1) Message-passing-based GNN layers that extracts the embedding of ROI nodes through iteratively updating information with structural connections. The propagation rule can be formulated in matrix form as: $H^{(l+1)} = GNN\left(A, H^{(l)}; \theta^{(l)}\right)$, where $H^{(l+1)} \in \mathbb{R}^{M \times D}$ are the embeddings computed after l step of the GNN layers, and D is the embedding dimension. GNN is the message propagation function using a combination of linear transformations and ReLU non-linearities, which depends on the adjacency matrix A, trainable parameters $\theta^{(l)}$, and the node embeddings $H^{(l)}$ generated from the previous step. The input node embeddings H^0 are initialized using the node features on the graph. 2) The graph pooling layer. It realizes the aggregation of global information at the graph level using readout to convert all node embeddings into a graph embedding vector. Here, the readout function can be performed using the average pool.

2.2 Functional Subdivision Block

Considering the heterogeneity of brain networks induced by intrinsic functional brain states, we propose to encode brain networks into multiple latent feature subspaces corresponding to functional brain states. The key to achieve this goal is to build an assignment matrix that can allocate the feature representation of each dimension in the brain network to the latent subspace related to distinct brain states.

Here, we innovatively design a learnable assignment method, which is determined by the embedding matrix and automatically updated with the training of the whole model. Specifically, we first utilize two separate GNN layers to generate embeddings for preliminary node feature matrix $H_F = GNN_{\text{feat}}\left(A, H; \theta_{feat}\right)$ and input embeddings of assignment matrix $H_S = GNN_{\text{assig}}\left(A, H; \theta_{assig}\right)$, respectively. Note that these two GNN layers use the same data as input, but have distinct parameterizations and play separate roles. We continue to transpose the input embeddings of assignment matrix as $H_S^T \in \mathbb{R}^{D \times M}$, and the generation of assignment matrix $S \in \mathbb{R}^{D \times C}$ as follows:

$$S = \text{softmax}\left(\text{MLP}_1\left(H_S^T\right)\right), \tag{1}$$

where the softmax function is applied in a row-wise fashion, and the output dimension of MLP_1 corresponds to a pre-defined number C of brain states.

With the assignment matrix and node embedding matrix in hand, we further extract distinct node embeddings in different latent subspaces corresponding to brain states. For each column $\{S_c\}_{c=1}^{C}$ in the assignment matrix, it is essentially a mask vector where each element represents the probability that the feature is assigned to the brain state c. Therefore, we can obtain the brain network representation in each brain state through the product of feature and its corresponding assignment probability.

$$H_{F_c} = \text{MLP}_2\left(H_F \odot \text{R}\{S_c\}^T\right), \tag{2}$$

where R is a repeat function that extends the mask vector to the same dimension of the node embedding matrix, $\odot$ denotes element-wise multiplication, and MLP_2 maps each new node embedding matrix to distinct feature latent subspaces, which characterize heterogeneous information under different brain states.

2.3 Functional Aggregation Block

After assigning the node embedding matrix of brain network into distinct latent subspaces, we utilize multiple GNN modules (each consists of a GNN layer and a graph pooling layer) to obtain the graph embedding of brain network $H_c \in \mathbb{R}^{1\times D}$ corresponding to each brain state respectively. These GNN layers are performed with shared weight to reduce the complexity of the model. Considering that each brain state has different contributions to the final brain network representation, we propose a functional aggregation block based on the self-attention mechanism to aggregate the information into a joint latent space, and acquire a comprehensive brain network representation for brain disorder diagnosis.

In practice, the graph embedding in every brain state is first packed together into a matrix $\{H_C|\{H_c\}_{c=1}^{C}, H_C \in \mathbb{R}^{C\times D}\}$ and then mapped into three matrices, including query $Q = H_C W_q$, key $K = H_C W_k$, and value $V = H_C W_v$, where the weight matrices for W_q, W_k, W_v are the learned linear mappings. Therefore, we can calculate the self-attention by mapping a query and a set of key-value pairs, and combining with a mean pooling to obtain the whole graph embedding vector $\widetilde{H} \in \mathbb{R}^{1\times D}$ for the brain network.

$$\widetilde{H} = \frac{1}{C}\sum_{c=1}^{C} \mathrm{softmax}(QK^T/\sqrt{D})V. \tag{3}$$

Here, the dot product is adopted to reduce computational and storage costs, softmax is used to normalize the self-attention and the scale $\sqrt{D}$ prevents the saturation led by softmax function. Finally, we fed the whole graph embedding vector into a fully connected layer to predict the diagnostic result $\hat{y}_n$.

2.4 Objective Function

In this work, we design an objective function composed of three components: First, we employ conventional supervised cross-entropy objective towards ground-truth y_n disorder prediction, defined as

$$\mathcal{L}_{\mathrm{CLF}} = -\frac{1}{N}\sum_{n=1}^{N} \left(y_n \log\left(\hat{y}_n\right) + \left(1-y_n\right)\log\left(1-\hat{y}_n\right)\right). \tag{4}$$

Second, since each row of the assignment matrix S_i represents the probability of allocating the feature of this dimension to different latent subspaces, it should generally be close to a one-hot vector, i.e., each dimension feature is assigned to each latent subspace. Therefore, we design an entropy loss to reduce the uncertainty of mapping distribution by minimizing entropy H_{S_i}:

$$\mathcal{L}_{\mathrm{E}} = \frac{1}{D}\sum_{i=1}^{D} H(S_i). \tag{5}$$

Finally, to ensure the generalization ability of the model and reduce over-fitting, we add an $L2$ normalization term. To summarize, the total loss of the proposed model can be formulated as: $\mathcal{L} = \mathcal{L}_{\mathrm{CLF}} + \alpha * \mathcal{L}_{\mathrm{E}} + \beta * L_2$, where α, β are hyper-parameters that determine the relative importance of feature fusion loss items.

3 Experiments

3.1 Dataset and Experimental Settings

We evaluate our framework on publicly available Alzheimer's Disease Neuroimaging Initiative (ADNI) dataset [16], which includes 193 normal controls (NC), 240 early mild cognitive impairment (EMCI), and 149 late mild cognitive impairment (LMCI). We use them to form three binary classification tasks abbreviated as N-E, N-L, and E-L. The fMRI data is preprocessed in a standardized protocol including slice time correction, motion correction, spatial and temporal filtering, and covariates regression [2]. We follow the general process of the GNN-based method in brain network analysis and use the AAL atlas [19] to define 90 ROIs for every subject. We continue to construct brain networks using Pearson correlations.

We compare our proposed model with five different methods, including one conventional model (1) SVM [6] where functional brain networks are reshaped as feature vectors and are then put into models, two representative GNN models: (2) GCN [12], (3) GAT [20], and two state-of-the-art GNN-based models specifically designed for brain networks: (4) BrainGNN [15] and (5) IBGNN [4].

All deep learning experiments are conducted on NVIDIA GeForce GTX TITAN X GPUs with PyTorch [17] framework. We perform a grid search to determine the better choice for $\alpha = 10^{-3}$ and $\beta = 10^{-2}$, and set parameter $c = 7$ representing different configurations of the brain as suggested in [1,8]. We refer readers of interest to supplementary materials for detailed experimental settings. All reported results are averaged across 10 times ten-fold cross-validations. We finally adopt four commonly used metrics to evaluate all methods, including classification accuracy (ACC), sensitivity (SEN), specificity (SPE), and AUC.

3.2 Result Analysis

Table 1 shows the classification results of all methods on all tasks. We can have the following observations. First, compared with the conventional machine learning method (i.e., SVM), deep learning models generally achieve better performance on all tasks in terms of four evaluation metrics. It is indicated that the brain features obtained by automatic learning with neural networks may be better than the traditional handcrafted features in the diagnosis of brain diseases. Second, two GNN models specifically designed for brain networks (i.e.,

BrainGNN, and IBGNN) achieve better results than classical GNN models (i.e., GCN, and GAT), demonstrating the significance of considering the biomedical characteristics of brain networks when applying GNN-related models to brain network analysis. Finally, the effectiveness of our design for heterogeneous properties of the brain network is demonstrated by its superior performance compared with other SOTA models. Moreover, our method is statistically significantly better than other methods (with $p < 0.05$) based on pairwise t-test. For instance, in terms of ACC values, the proposed LSGNN obtains the improvement of at least 3% compared with the best alternatives (i.e., IBGNN) on all tasks. It is concluded that LSGNN is feasible to separate the heterogeneous feature of brain networks in latent space, which is beneficial to capture complex information through multiple GNN modules under distinct brain states, thus improving the ability of brain network representation.

Table 1. Classification results (mean ± std) of all methods on three tasks (%).

Tasks	Metrics	SVM	GCN	GAT	BrainGNN	IBGNN	LSGNN
N-E	ACC	$65.82_{\pm 1.23}$	$69.35_{\pm 1.39}$	$71.20_{\pm 1.11}$	$74.31_{\pm 1.48}$	$75.79_{\pm 1.39}$	$\mathbf{78.88}_{\pm 1.58}$
	SEN	$58.78_{\pm 1.34}$	$69.42_{\pm 1.85}$	$72.33_{\pm 1.75}$	$73.29_{\pm 1.80}$	$74.95_{\pm 2.13}$	$\mathbf{76.52}_{\pm 1.66}$
	SPE	$67.92_{\pm 1.28}$	$65.28_{\pm 1.44}$	$65.37_{\pm 1.28}$	$66.24_{\pm 1.92}$	$67.12_{\pm 1.03}$	$\mathbf{68.52}_{\pm 1.49}$
	AUC	$66.16_{\pm 1.33}$	$70.97_{\pm 1.71}$	$72.15_{\pm 1.29}$	$73.12_{\pm 1.30}$	$74.89_{\pm 1.86}$	$\mathbf{79.42}_{\pm 1.53}$
N-L	ACC	$69.14_{\pm 1.11}$	$74.52_{\pm 1.72}$	$75.49_{\pm 1.81}$	$82.34_{\pm 1.14}$	$82.90_{\pm 2.32}$	$\mathbf{87.47}_{\pm 1.71}$
	SEN	$62.48_{\pm 1.08}$	$79.77_{\pm 1.28}$	$78.34_{\pm 1.19}$	$79.21_{\pm 1.99}$	$78.10_{\pm 2.25}$	$\mathbf{81.58}_{\pm 1.52}$
	SPE	$72.92_{\pm 1.14}$	$75.98_{\pm 1.92}$	$75.48_{\pm 2.42}$	$78.12_{\pm 1.23}$	$77.85_{\pm 2.11}$	$\mathbf{79.86}_{\pm 1.33}$
	AUC	$71.45_{\pm 1.12}$	$76.59_{\pm 1.54}$	$74.29_{\pm 1.66}$	$78.74_{\pm 1.39}$	$79.12_{\pm 2.50}$	$\mathbf{83.15}_{\pm 1.55}$
E-L	ACC	$62.95_{\pm 1.14}$	$66.53_{\pm 2.20}$	$65.49_{\pm 2.30}$	$67.62_{\pm 2.25}$	$70.23_{\pm 1.95}$	$\mathbf{74.24}_{\pm 1.64}$
	SEN	$61.63_{\pm 1.09}$	$68.42_{\pm 1.94}$	$68.12_{\pm 2.89}$	$68.33_{\pm 1.93}$	$68.81_{\pm 1.69}$	$\mathbf{70.55}_{\pm 1.59}$
	SPE	$64.40_{\pm 1.05}$	$62.87_{\pm 2.37}$	$64.16_{\pm 1.97}$	$61.59_{\pm 2.61}$	$62.49_{\pm 1.30}$	$\mathbf{65.37}_{\pm 1.39}$
	AUC	$61.48_{\pm 1.10}$	$62.95_{\pm 1.98}$	$63.28_{\pm 2.21}$	$64.82_{\pm 2.10}$	$67.39_{\pm 1.51}$	$\mathbf{70.08}_{\pm 1.48}$

3.3 Ablation Study

We conduct ablation studies to verify the effectiveness of 1) the learnable assignment method in the FSB module, 2) the self-attention mechanism-based fusion method in the FAB module, and 3) entropy loss $\mathcal{L}_{\mathrm{E}}$. Specifically, In the FSB module, we compare the proposed learnable method with a fixed method, where we utilize k-means to cluster feature embedding into several latent subspaces with the same number as the learnable assignment matrix done. In the FAB module, we try a typically simple feature fusion method (i.e., feature concatenation) without self-attention. For the loss function, we conduct comparative experiments on whether to include entropy loss. The classification results of all six methods on the N-E task are listed in Table 2. It can be observed that the proposed learnable assignment method and self-attention mechanism-based fusion module are effective in cognitive disorder diagnosis. Furthermore, the results of

entropy loss ablation prove that the introduction of entropy loss greatly enhances the robustness of the proposed model.

Table 2. Ablation study of LSGNN with different modules on N-E task.

FSB		FAB		Loss		Metrics		
Learnable	Fixed	Self-Att	Concat	$\mathcal{L}_{\mathrm{E}}$	Without	ACC	SEN	SPE
√		√		√		**78.88**$_{\pm 1.58}$	**76.52**$_{\pm 1.66}$	**68.52**$_{\pm 1.49}$
√		√			√	74.18$_{\pm 3.38}$	72.23$_{\pm 2.72}$	64.12$_{\pm 3.19}$
√			√	√		76.42$_{\pm 1.82}$	75.82$_{\pm 1.71}$	66.39$_{\pm \mathbf{1.13}}$
√			√		√	74.20$_{\pm 3.41}$	72.11$_{\pm 2.59}$	65.86$_{\pm 2.98}$
	√	√			√	72.30$_{\pm 2.19}$	71.12$_{\pm 1.74}$	64.23$_{\pm 2.45}$
	√		√		√	71.93$_{\pm 2.04}$	71.27$_{\pm 1.98}$	65.23$_{\pm 1.79}$

3.4 Interpretability of Brain States

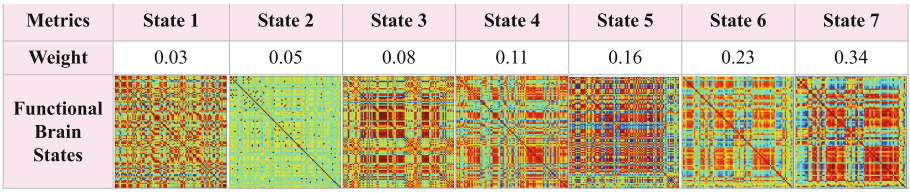

Fig. 2. Interpretability analysis of brain network in distinct brain states on N-E task.

To investigate brain states and revealing the impact of different brain states on diseases, we plot the functional brain states under distinct brain network feature subspaces on the N-E task. Specifically, we first calculate the assignment matrix using Eq. 2 and further compute the sum of each column combined with normalization. Each element is the probability weight of each brain state in the whole feature space, which also reflects the impact of each brain state on the final diagnosis task. The weight values of different brain states are sorted in the second line in Fig. 2. It is evident that the divergence of the impacts from distinct brain states is significant. For example, the weight of state 7 surpasses that of state 1 by over 10 times. The possible reason is that the heterogeneous functions (e.g. Visual, Attention, Memory, etc.) conferred from distinct brain states may have unequal contributions to the cognitive activities.

Then, for each brain state c, we extract node embedding matrix H_{F_c} and construct a corresponding functional connectivity matrix using Pearson correlation. Finally, we obtain distinct brain states by computing the average results of testing samples on the N-E task. From Fig. 2, we have an interesting observation

that the brain state that has a great impact on diagnosis shows rich club regions, which reveals that there exist multiple subnetworks in the brain network that may correlate to different brain functions.

4 Conclusion

In this paper, we propose a novel learnable subdivision graph neural network method for functional brain network analysis and interpretable cognitive disorder diagnosis. Specifically, brain networks are embedded into multiple latent feature subspaces corresponding to functional configurations in a learnable way. Experimental results of the cognitive disorder diagnosis tasks verify the effectiveness of our proposed method. A direct future direction based on this work is to utilize heterogeneous graph construction techniques to describe brain network patterns. This allows for consideration of brain network heterogeneity from the initial step of brain network modeling, which could lead to a better understanding of brain networks.

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