Joint Embedding of Structural and Functional Brain Networks with Graph Neural Networks for Mental Illness Diagnosis

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Background

Background: Brain Network Analysis

- Brain network analysis is shown effective in mental health analysis.
- Brain networks representing complex structures of human brain connectivities are important for understanding biological mechanisms of brain functions.
- Different modalities of brain networks provide complementary information to each other and joint utilizing multiple modalities often leads to consistent improvement.

Challenges of Applying Deep Graph Neural Networks in Multiview Brain Network Analysis

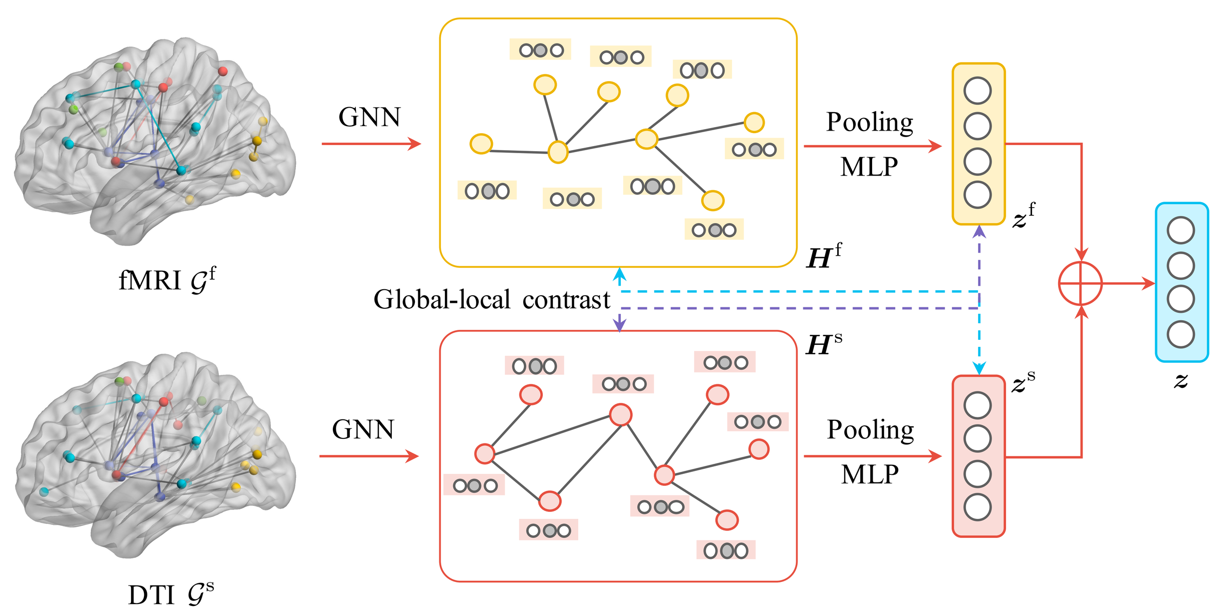
- Different modalities encode different biomedical semantics of brain regions.
- Most brain networks are organized in a form of weighted adjacency matrix describing connections among brain regions without initial node features.

Joint Embedding of Structural and Functional Brain Networks with GNNs

Technical Highlights

We propose a novel BrainNN framework that jointly embeds multimodal brain networks with message passing GNNs:

- **Multimodal fusion.** We treat the brain networks under different modalities as multiple views of the brain and resort to contrastive learning for jointly embedding structural and functional brain networks.
- **Message-passing-based GNNs.** We derive statistical node attributes from original multimodal data and leverage a general message passing GNN model to properly embed edge weights into learned node representations.



Multimodal Fusion across Multiple Views

We employ a contrastive objective that distinguishes node representations of one view with graph representations of the other and vice versa [1, 2]:

$$\mathcal{J}_{\text{con}} = \frac{1}{2S}\sum_{\mathcal{G}_i\in\mathcal{M}}\left[\frac{1}{N}\sum_{v_i\in\mathcal{V}}\left(I(\boldsymbol{h}_i^{\text{f}}; \boldsymbol{z}_i^{\text{s}}) + I(\boldsymbol{h}_i^{\text{s}}; \boldsymbol{z}_i^{\text{f}})\right)\right]. \tag{1}$$

We estimate the mutual information $I(X;Y)$ in Eq. (1) using Jason-Shannon Divergence (JSD) [3]:

$$I(\boldsymbol{h}_i;\boldsymbol{z}_i) = -\mathrm{sp}(-d(\boldsymbol{h}_i,\boldsymbol{z}_i)) - \frac{1}{N-1}\sum_{v_j\in\mathcal{V}\backslash\{v_i\}}\mathrm{sp}(d(\boldsymbol{h}_i,\boldsymbol{z}_j)). \tag{2}$$

Joint Embedding of Structural and Functional Brain Networks with GNNs (cont.)

Message Passing GNNs for Brain Networks

Constructing node features for modality graphs. Existing local statistical measures are known to improve expressiveness of GNNs. We compute local degree profiles (LDP) [4] for each brain modality, where each feature $\boldsymbol{x}_n$ of modality graph $\mathcal{G}_{ij}$ is computed as

$$\boldsymbol{x}_n = [\deg(n); \min(\mathcal{D}_n); \max(\mathcal{D}_n); \mathrm{mean}(\mathcal{D}_n); \mathrm{std}(\mathcal{D}_n)]. \tag{3}$$

Implementing message passing GNN for handling edge weights. Since the brain region connectivity is expressed in edge weights, we first construct a message vector $\boldsymbol{m}_{ij}$ composed of node embeddings of a node i, its neighborhood j, and edge weights w_{ij}:

$$\boldsymbol{m}_{ij}^{(l)} = t_\Theta\left(\left[\boldsymbol{h}_i^{(l)}; \boldsymbol{h}_j^{(l)}; w_{ij}\right]\right). \tag{4}$$

Then, we aggregate messages from all neighborhoods followed by a non-linear transformation:

$$\boldsymbol{h}_i^{(l)} = \sigma\left(\sum_{j\in\mathcal{N}_i\cup\{i\}} \boldsymbol{m}_{ij}^{(l-1)}\right). \tag{5}$$

Finally, we employ a MLP with residual connections to summarize all node embeddings to compute graph embeddings $\boldsymbol{z}$:

$$\boldsymbol{z}' = \sum_{i\in\mathcal{V}} \boldsymbol{h}_i^{(k)}, \qquad \boldsymbol{z} = t_\Phi(\boldsymbol{z}') + \boldsymbol{z}'. \tag{6}$$

Experiments

Method	HIV		BP	
	Accuracy	AUC	Accuracy	AUC
M2E	50.61	51.53	57.78	53.63
MIC	55.63	56.61	51.21	50.12
MPCA	67.24	66.92	56.92	56.86
MK-SVM	65.71	68.89	60.12	56.78
3D-CNN	74.31	73.53	63.33	61.62
GAT	68.58	67.31	61.31	59.93
GCN	70.16	69.94	64.44	64.24
DiffPool	71.42	71.08	62.22	62.54
MVGCN	74.29	73.75	62.22	62.64
V-GCN	70.00	75.83	67.14	61.17
CONCAT	66.36	72.39	67.27	61.13
BrainNN	**77.14**	**79.79**	**73.64**	**67.54**

Table 1. Overall performance and ablation studies

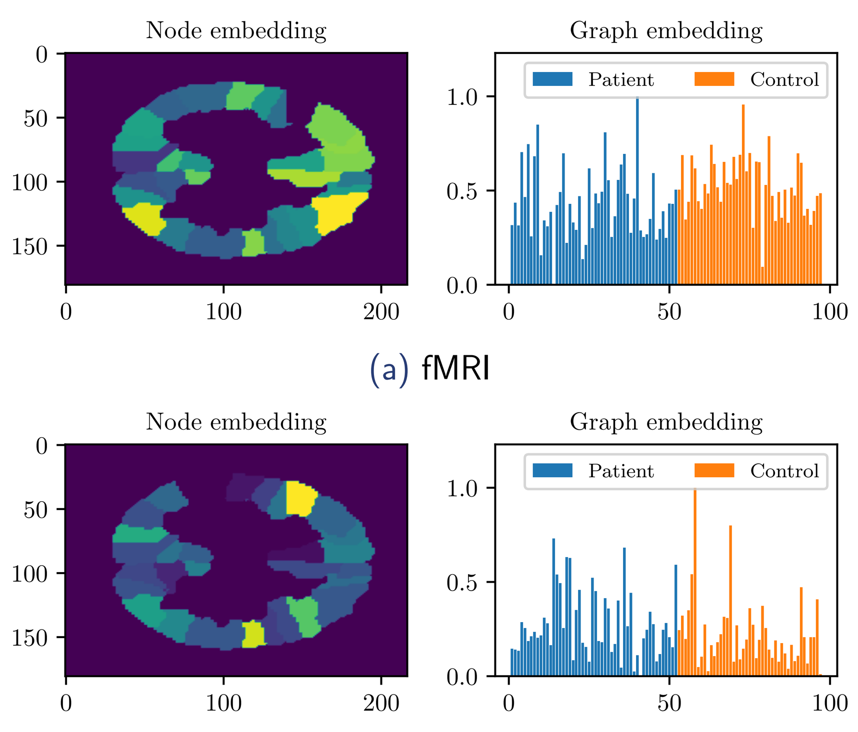


Figure 1. Visualization of embedded features

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