Exploring Spatio-Temporal Interpretable Dynamic Brain Function with Transformer for Brain Disorder Diagnosis

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Abstract. The dynamic variation in the spatio-temporal organizational patterns of brain functional modules (BFMs) associated with brain disorders remains unclear. To solve this issue, we propose an end-to-end transformer-based framework for sufficiently learning the spatio-temporal characteristics of BFMs and exploring the interpretable variation related to brain disorders. Specifically, the proposed model incorporates a supervisory guidance spatio-temporal clustering strategy for automatically identifying the BFMs with the dynamic temporal-varying weights and a multi-channel self-attention mechanism with topology-aware projection for sufficiently exploring the temporal variation and spatio-temporal representation. The experimental results on the diagnosis of Major Depressive Disorder (MDD) and Bipolar Disorder (BD) indicate that our model achieves state-of-the-art performance. Moreover, our model is capable of identifying the spatio-temporal patterns of brain activity and providing evidence associated with brain disorders. Our code is available at https://github.com/llt1836/BISTformer.

Keywords: Dynamic Brain Networks · Spatio-Temporal Transformer · Bipolar Disorder · Major Depressive Disorder · Functional Magnetic Resonance Imaging (fMRI)

1 Introduction

Dynamic brain function analysis based on rs-fMRI data plays an important role in understanding human brain organization and recovering the pathology and activity variation when suffering from brain disorders [16,20,25]. It is generally believed that dynamic brain activity inherently reflects the temporal collaboration of brain functional modules (BFMs) which are considered as clusters

of brain regions with strong internal coupling and weak external coupling and flexibly combine with each other at different time points for different cognitive demands [3,25]. Although some works have improved predictive performance through learning the brain activity from dynamic functional connectivity (dFC) and provided some insights into the etiology of brain disorders [2,4,11,28], they neglected *the identification of BFMs and the exploration of their collaborative relationships to reveal the inherently disorder-related spatio-temporal characteristics in brain dynamics*. There are three critical challenges that need to be solved in modeling the disorder-related BFMs with spatio-temporal clustering for learning dynamic brain activity: 1) how to design the supervised cluster strategy for identifying the inherent topology structure of the BFMs under the classification, 2) how to concurrently build spatio-temporal clustering and capture the latent spatio-temporal representation of brain dynamics, and 3) how to establish the mapping between the collaboration among BFMs and brain disorders for providing spatio-temporal interpretability.

To solve the aforementioned issues, we propose an end-to-end **I**nterpretable transformer-based framework for joint training of **S**patio-**T**emporal clustering and feature learning for **B**rain disorder diagnosis, named BISTformer. Firstly, we propose to cluster multiple collaboratively interacting BFMs with the corresponding temporal-varying weights from the dFCs through tensor decomposition. The self-attention mechanism is employed to learn the temporal variation for capturing the temporal-varying weights under the various channels of BFMs. We also propose a reconstruction loss with several regularization terms to appropriately constrain the integration of the diverse BFMs. To sufficiently model the representation of dynamic brain activity, a topology-aware projection layer is involved in the process of graph convolution. We evaluate our model on two real medical clinical applications: Bipolar Disorder (BD) diagnosis and Major Depressive Disorder (MDD) diagnosis. The experimental results demonstrate the improvement of our model. Moreover, the interpretable analysis reveals the spatio-temporal patterns related to MDD and BD discovered by our model. Our contributions are summarized as follows:

- We propose an end-to-end spatio-temporal interpretable transformer-based framework for dynamic brain activity analysis.
- We propose a classification-guided clustering with tensor decomposition for capturing disorder-related spatio-temporal organization.
- The experimental results demonstrate that BISTformer generally outperforms in various brain disorders diagnosis, such as MDD and BD.

2 Method

The framework of our proposed model is shown in Fig. 1. We first decompose dynamic brain function into BFMs and corresponding temporal-varying weights by spatio-temporal clustering. In each BFM channel, self-attention with the proposed topology-aware projection through graph convolution is employed

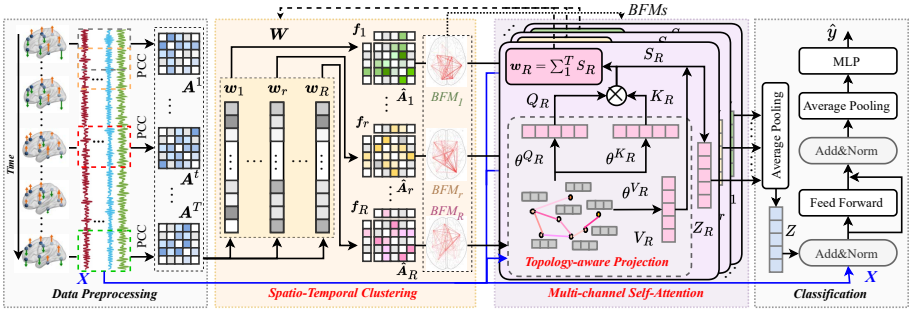

Fig. 1. The overall architecture of our proposed BISTformer framework.

for adaptively learning the temporal variation and sufficiently capturing spatio-temporal representation. Finally, the remaining transformer encoder layer and MLP are employed to further obtain the spatio-temporal feature and obtain satisfactory performance. In addition, through clustering on the temporal-varying weights, we divide the temporal variation into two states. The active state consists of a few crucial time points that provide more discriminate spatio-temporal information when diagnosing. Besides, we assess the contributions of BFMs to diagnosis by progressively removing them and providing neurological evidence by mapping them with Intrinsic Connectivity Networks (ICNs).

2.1 Spatio-temporal Clustering for BFMs Identification

To explore the spatial distribution of BFMs and understand their collaborative relationships, we treat the spatio-temporal clustering for BFMs identification as a CANDECOMP/PARAFAC (CP) decomposition model [25], which decomposes the dynamic brain function as a sum of rank-one tensors. Specifically, we introduce a learnable parameter $\boldsymbol{F} \in \mathbb{R}^{R \times M}$ optimized for clustering the M ROIs to the various R BFMs and each item $f_{r,m}$ of $\boldsymbol{F}$ denotes the membership of the ROI m to the r-th BFM. Then, we approximately reconstruct the dFCs by the linear combination of several BFMs with the corresponding temporal-varying weights as follows:

$$L_{rec} = argmin_{\boldsymbol{f}_r} \sum_{i=1}^{N} \sum_{t=1}^{T} \left\| \boldsymbol{A}_i^t - \sum_{r=1}^{R} \boldsymbol{f}_r \circ \boldsymbol{f}_r \circ w_{r,t}^i \right\|_F^2 \tag{1}$$

where N is the number of subjects, $\boldsymbol{A}_i^t \in \mathbb{R}^{M \times M}$ is the adjacent matrix of t-th dFC, and $\circ$ is the vector outer product. The topological structure of r-th BFM can be defined as $\hat{\boldsymbol{A}}_r = \boldsymbol{f}_r \circ \boldsymbol{f}_r$, $\boldsymbol{f}_r \in \mathbb{R}^{1 \times M}$, $\hat{\boldsymbol{A}}_{\boldsymbol{r}} \in \mathbb{R}^{M \times M}$. Importantly, $w_{r,t}^i$ is the element of the temporal-varying weights $\boldsymbol{W} \in \mathbb{R}^{N \times R \times T}$ optimized in the self-attention module under the r-th BFM as illustrated in Section 2.2.

2.2 Multi-channel Spatio-Temporal Transformer for temporal variation modeling and representation learning

Inspired by the exciting success of the transformer [22] in the time series analysis task, we employ it to model the dynamic brain activity and capture the temporal-varying weights. We perform self-attention independently for the multiple channels of BFMs leading to a more expressive model that excels in capturing diverse dynamic dependencies semantic and activity patterns related to the brain disorders in fMRI data.

Topology-aware Projection: Considering that the transformer only captures temporal attributed similarity but cannot identify structural differences among tokens [5], we proposed a topology-aware projection with graph convolution to learn sufficient spatio-temporal representation. Specifically, the projection process of each channel for generating query, key, and value is as follows:

$$Q_r, K_r, V_r = ReLU\left(\left|\tilde{\boldsymbol{D}}_r{}^{-1/2}\tilde{\boldsymbol{A}'}_r\tilde{\boldsymbol{D}}_r{}^{-1/2} \odot X^t\right|_1^T \theta_r^Q, \theta_r^K, \theta_r^V\right) \tag{2}$$

where X^t is the BOLD signals of all ROIs at time point t, $\tilde{\boldsymbol{A}'}_r = \hat{\boldsymbol{A}}_{\boldsymbol{r}} + \boldsymbol{I}$ is the adjacent matrix of the r-th BFM and $\tilde{\boldsymbol{D}_{r,ii}} = \sum_j \tilde{\boldsymbol{A}'}_{r,ij} \in \mathbb{R}^{M\times M}$. $|\cdot|_1^T$ denotes the concatenation for merging features from different time points. $\theta_r^Q \in \mathbb{R}^{D\times D_Q}$, $\theta_r^K \in \mathbb{R}^{D\times D_K}$, and $\theta_r^V \in \mathbb{R}^{D\times D_V}$ are the learnable parameters.

Temporal-varying weights Learning: After projection, the temporal-varying weight $\boldsymbol{w}_r \in \mathbb{R}^{N\times T}$ in the r-th channel for modeling the temporal variation is calculated as follows:

$$\boldsymbol{w}_r = \sum_{t=1}^{T} S_r = \sum_{t=1}^{T} softmax\left(Q_r K_r^{\mathrm{T}}/\sqrt{D_Q}\right) \tag{3}$$

The incorporation of the multiple channels' features enables our model to be sensitive to the diverse contributions of BFMs for brain disorder diagnosis simultaneously. The final spatio-temporal feature is obtained as follows:

$$Z = ReLU\left(LN\left(X + AvgPool\left(S_r V_r\right)\right)\theta_1\right)\theta_2 \tag{4}$$

where $\theta_1 \in \mathbb{R}^{d\times D}$ and $\theta_2 \in \mathbb{R}^{d\times D}$ are the learnable parameters in the feed-forward network. $LN\left(\cdot\right)$ is the Layer normalization.

2.3 Joint learning

Optimizing the clustering and classification jointly can substantially improve the performance of both in exploring disease-related dynamic brain activity. Moreover, we introduced several regularization terms to prevent overfitting of our model and assign the brain regions to different BFMs appropriately. Finally, our objective function is defined as:

$$L = L_{cls} + \lambda_1 L_{rec} + \lambda_2 L_{r1} + \lambda_3 L_{r2} + \lambda_4 L_{r3} \tag{5}$$

where L_{cls} is the cross-entropy loss, $L_{r1} = \sum_{r=1}^{R} \left\| \boldsymbol{f}_r \circ \boldsymbol{f}_r - diagonal(\boldsymbol{f}_r^2) \right\|_F$ is orthogonal regularization to penalize the off-diagonal elements of $\hat{\boldsymbol{A}}_r$ for hindering the overlap among different BFMs, $L_{r2} = \sum_{r=1}^{R} Variance(\boldsymbol{f}_r^2)$ is a balancing regularization to achieve a balanced distribution for better interpretability, $L_{r3} = \sum_{r=1}^{R} RELU(-\boldsymbol{f}_r)$ is to guarantee the values of $\boldsymbol{f}_r$ are positive. λ_1, λ_2, λ_3 and λ_4 are the trade-off hyper-parameters.

It is noteworthy that the temporal-varying weights $\boldsymbol{W}$ obtained from the multi-channel self-attention are accepted as the input of the clustering module when updating $\boldsymbol{F}$. Meanwhile, the spatio-temporal clustering also impacts the computation of $\boldsymbol{W}$ as the computation operates at multiple channels corresponding to various BFMs. Hence, the optimization of our objective function inherently involves an alternating training process. For simplicity, following [18], we adopt the approximate joint training for parameter updating. In each iteration, the clusters of BFMs are generated and fixed when calculating $\boldsymbol{w}_r$ in each channel of BFM during forward propagation. The backward propagation takes place as usual under the supervision of L, i.e. the clustering and the classification are performed simultaneously.

3 Experiments and Interpretation

3.1 Dataset and experimental details.

We implemented experiments by 10-fold cross-validation on a private dataset constructed from Nanjing Medical University (NMU) for MDD and BD diagnosis. The dataset includes 246 health controls (152 females and 94 males, aged 26.7±6.1 years), 151 MDDs (108 females and 43 males, aged 17.0±5.0 years), and 126 BDs (83 females and 43 males, aged 17.2±4.0 years). The preprocessing includes spatial normalization with echo planar imaging (EPI) template of standard Montreal Neurological Institute (MNI) space (spatial resolution 3 mm×3mm×3 mm), spatial and temporal smoothing with a 6 mm×6mm×6 mm Gaussian kernel and filter processing with 0.01-0.08Hz low-frequency fluctuations for removing interference signals. The Automated Anatomical Labeling (AAL-116) atlas is used for extracting ROIs.

3.2 Results and Discussion

Comparison with state-of-the-art Methods: Two types of methods are compared including single-domain and spatio-temporal domain methods. As shown in Table 1, the proposed model obtains state-of-the-art classification results under our consideration with statistical significance. The results indicate that modeling the BFMs and learning the temporal variation is indeed beneficial for learning dynamic brain activity related to brain disorders. Our model is effective in brain disorder diagnosis.

Ablation study: We also individually reduced the proposed modules (-w/o SA: without self-attention, -w/o JL: without joint learning, -w/o STC: without

Table 1. The comparison with state-of-the-art methods. The best results are boldfaced. p is the Student's t-test level. ($*$: 0.01< p <0.05, † : 0.001< p <0.01, ‡ : p <0.001)

Methods	MDD vs. HC			BD vs. HC		
	ACC%	**AUC%**	**F1%**	**ACC%**	**AUC%**	**F1%**
BrainNetCNN [12]	67.9±6.7‡	65.8±7.9‡	67.2±3.8‡	68.8±4.5‡	64.5±7.7‡	66.3±8.2‡
ASD-DiagNet [10]	66.8±1.4‡	62.4±5.7‡	65.5±2.1‡	71.2±5.6‡	70.1±3.7‡	70.9±1.9‡
GroupINN [27]	64.5±2.9‡	63.6±5.4‡	64.9±0.9‡	65.9±2.1‡	61.2±5.1‡	66.4±3.7‡
BrainGNN [15]	66.5±5.5‡	64.1±1.8‡	66.5±3.1‡	68.3±1.1‡	66.9±7.1‡	67.5±2.8‡
MVS-GCN [24]	69.7±3.2‡	68.1±2.2‡	68.4±7.3‡	71.2±0.4‡	69.8±2.4‡	69.4±5.8‡
LSTM-ASD [8]	69.8±5.7‡	67.7±4.8‡	65.7±9.4‡	68.4±6.2‡	68.1±4.6‡	69.9±8.7‡
GC-LSTM [26]	69.2±3.9‡	68.7±2.7‡	66.3±8.3‡	69.8±2.8‡	68.3±1.7‡	68.6±4.7‡
GSA-LSTM [4]	68.4±5.3‡	67.9±4.3‡	65.3±6.8‡	70.1±3.5‡	69.1±4.3‡	67.9±4.1‡
ST-GCN [9]	58.0±7.5‡	52.6±7.2‡	53.9±7.1‡	65.3±6.4‡	57.4±8.1‡	62.3±6.2‡
TCN-GCN [1]	62.6±6.1‡	59.9±8.1‡	58.2±6.7‡	65.9±5.3‡	62.3±4.2‡	65.7±7.1‡
STAGIN [13]	63.5±3.8‡	61.4±4.1‡	59.3±7.1‡	65.8±3.6‡	63.7±4.4‡	63.2±6.9‡
BoLT [2]	72.5±2.2‡	70.2±1.9‡	68.6±7.4‡	70.1±2.1‡	69.3±2.3‡	67.9±12.2‡
ST-Transformer [7]	73.1±1.2‡	70.8±2.7‡	71.4±5.4‡	72.9±2.0‡	70.1±2.7‡	69.5±3.8‡
-w/o SA	68.3±4.4‡	68.9±3.7‡	64.4±5.9‡	66.8±5.2‡	67.2±3.2‡	65.5±3.9‡
-w/o JL	72.5±3.9‡	71.3±3.9‡	70.6±4.1‡	73.3±3.5‡	71.0±3.3‡	69.7±4.9‡
-w/o TWP	74.9±4.1†	73.8±3.3†	72.9±7.2‡	75.1±2.4*	72.3±2.6*	72.5±6.6‡
-w/o STC	74.7±5.8†	74.2±5.3†	73.2±5.2*	74.6±4.1†	71.6±3.0‡	73.1±6.6†
BISTformer	**76.6±1.4**	**75.8±2.3**	**74.6±4.8**	**76.3±2.5**	**73.7±2.9**	**74.5±6.4**

spatio-temporal clustering, -w/o TWP: without topology-aware projection) from BISTformer to verify the effectiveness of each component. From Table 1, we can conclude that the proposed components are necessary and complementary since they can work collaboratively and bring positive contributions to the learning of discriminating spatio-temporal features associated with brain disorders.

In addition, we demonstrate that our model achieves optimal performance when the number of BFMs is set to 8. All the experiments were conducted based on the configuration of 8 BFMs in total. Moreover, the trade-off parameters in the objective function are tuned through the validation set from a fixed range. The discussion of these parameters showed our model's robustness.

3.3 Spatio-Temporal Interpretation

Temporal states Identification: To explore the temporal expression and organization of dynamic brain function, we applied the K-means clustering with 3 clusters (determined by consideration of both the Calinski-Harabasz Index and the Silhouette Coefficient [23]) on the temporal-varying weights $\boldsymbol{W}$. As shown in Fig. 2, the clusters can be split into active (State1, State3) or stable (state2) states. The active state consists of time points with a larger phase difference, while the stable holds the opposite performance. We also calculate the fractional occupancy (FO) of each state, and the time spent in the stable state is significantly more than that in the active state (FO: 84.24% : 15.76% in MDD vs.

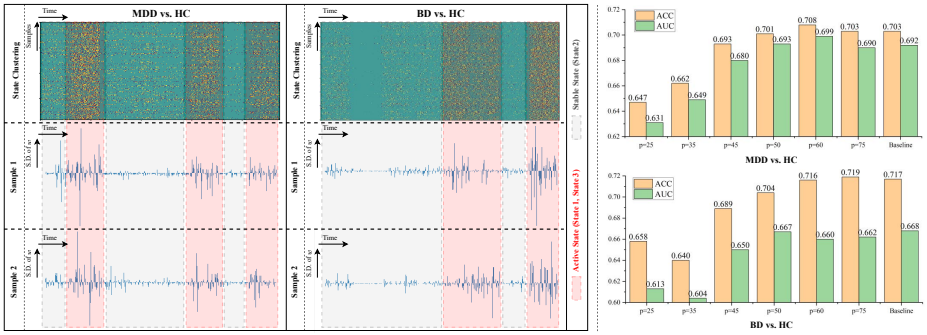

Fig. 2. The state splitting in MDD vs. HC and BD vs. HC datasets (left) and the performance with the active state under various $p\%$ (right).

HC/FO: 85.63% : 14.37% in BD vs.HC). It suggests that the dynamic brain function may indeed be driven at a few critical time points instead of the whole period, which is consistent with the previous studies [16,19], and the active state provides more discriminate spatio-temporal information when performing classification.

In addition, we also apply the classification by a transformer encoder trained by the BOLD signals in the whole period (Baseline) and the selected active state, separately. Since the state's transition exhibits approximate discernible periodicity and consistency across subjects, we determine whether a time point is active or stable through a voting mechanism. If more than $p\%$ subjects consider the point as stable, it is determined as stable, otherwise active. From Fig. 2, we can observe that when p=50 (MDD vs. HC) / p=60 (BD vs. HC), the performance significantly approximates the baseline. The results indicate that even after excluding certain time points of the stable state, the classification performance remains at par with the baseline, further substantiating the aforementioned findings.

Analyzing the Mapping between BFMs and Brain Disorders: We also conducted experiments to investigate the contributions of different BFMs to the diagnosis of brain disorders. Based on the aforementioned temporal states partitioning, we first generated some new datasets by removing the brain regions of one or more BFMs at the selected active state (MDD: p=50, BD: p=60). Then, we treated these datasets as inputs for training the basic transformer encoder to perform classification. As shown in Fig. 3, we can observe that the removal of BFM1, BFM4, and BFM7 leads to stable performance, even a slight increase in the classification results, whereas the performance shows a significant decline when removing BFM3, BFM5, and BFM8. It indicates that the dynamics of BFM3, BFM5, and BFM8 contribute significantly to the diagnosis of MDD, and their collaboration changes are associated with the onset of MDD. From Fig. 3, a similar observation can also be found when applying BD diagnosis, which means that BFM5 and BFM8 are more relevant to the occurrence of BD.

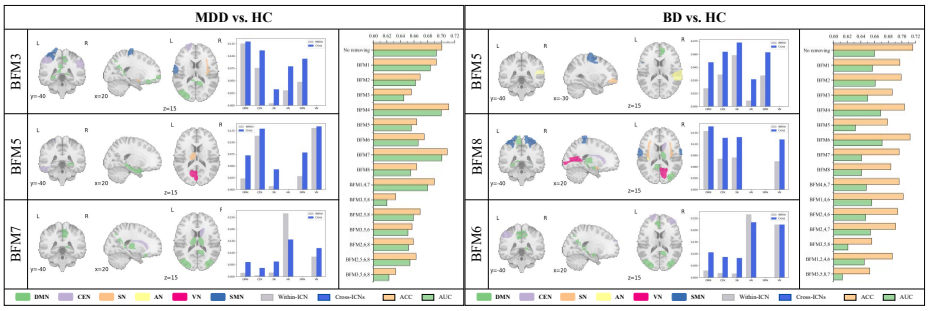

Fig. 3. The spatial distribution and corresponding connection strength of the top2 and last1 BFMs related to MDD and BD. The brain regions with various colors represent the different ICNs. The classification results under the removal of various BFMs are shown in the bar.

Furthermore, to quantify the functional relevance of BFMs with the known neurobiological knowledge, we evaluate six Intrinsic Functional Networks (ICNs) including DMN (default mode network), AN (auditory network), SN (salience network), SMN (somatomotor network), VN (visual network), CEN (central executive network) [14]. Since each item of $\boldsymbol{F}$ can reflect the membership of each brain region to the BFMs, we employ it to evaluate the within-ICN and cross-ICNs connection strength in each BFM according to [27]. The topology of the top 2 and last 1 BFMs and the corresponding strength scores are summarized in Fig. 3. The results demonstrate that MDD is associated with the altered functional connectivity of DMN, VN, and SN. On the contrary, CEN, DMN, and SN are hypothesized to be central to the symptomatology of BD. These findings are consistent with previous studies [6,17,21].

4 Conclusion

The dynamic brain function analysis for brain disorder diagnosis always ignores the spatio-temporal interpretation. To uncover the underlying dynamic roots of brain disorders, we propose an end-to-end joint training spatio-temporal clustering and feature learning framework based on transformer for modeling the temporal variation and brain function modules. The experiments on the NMU dataset for MDD and BD diagnosis demonstrate that our model achieves state-of-the-art performance. Besides, our model can identify the spatio-temporal patterns associated with brain disorders. The temporal states and biomarker findings can be confirmed by previous studies in neuroscience.

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