Brain-TM: Decoding Brain States from Functional Networks Using a Hierarchical Spatiotemporal Transformer-Mamba

Xuan Liu, Xuhui Wang, Sigang Yu, Di Zhu, Yincheng Yao, Shu Zhang✉

Center for Brain and Brain-Inspired Computing Research, School of Computer Science, Northwestern Polytechnical University, Xi'an, China.
shu.zhang@nwpu.edu.cn

Abstract. Understanding the dynamic transitions of brain states is crucial for comprehending the working mechanisms of the brain. However, accurately decoding these states from functional networks remains challenging, as existing methods lack the interpretability to reveal how internal hubs drive brain integration. To address this issue, we propose Brain-TM, a hierarchical Transformer-Mamba framework designed to decode brain states from functional networks. Evaluated on the HCP dataset across 7 cognitive tasks, Brain-TM achieves a superior classification accuracy of 94.7%. Beyond its predictive performance, it offers a biologically interpretable framework by proceeding at three analytical levels. Firstly, we identify task-specific network representations, demonstrating that latent brain states correspond to distinct cognitive demands across varying temporal windows. Secondly, we reveal a hub-based mechanism across brain states, showing that global network integration is fundamentally orchestrated by localized hub activations. Finally, we investigate the topological characteristics of functional hubs, validating their dominance via centrality metrics and benchmark comparisons. In summary, Brain-TM successfully decodes spatiotemporal dynamics, revealing that internal hubs play a pivotal role in driving brain states.

Keywords: Brain States · Brain Functional Networks · Brain Hubs · Transformer · Mamba.

1 Introduction

The human brain functions as a complex system, orchestrating information processing through the coordinated interplay among brain regions [1]. However, traditional static functional connectivity (sFC) averages neural activity over the entire scan, overlooking temporal variations in functional interactions[2]. Consequently, it overlooks the substantial temporal variations inherent in brain activity. To address this limitation, recent research has adopted dynamic functional connectivity (dFC) to characterize these time-varying connectivity patterns [3]. Analysis of dFC reveals that the brain transitions among distinct, recurrent

configurations known as brain states [4]. These states are widely recognized as intrinsic neural substrates that support diverse cognitive functions [5, 6].

These dynamic states arise from the flexible organization of functional networks (FNs) [7]. Critically, whole-brain communication relies on specific key regions known as hubs, which are highly connected nodes that facilitate information flow between different brain areas [8, 9]. For instance, the activity of hubs within the Frontoparietal and Default Mode Networks is essential for cognitive flexibility [10]. Therefore, to accurately decode and understand brain states, models must be capable of capturing the complex spatiotemporal organization of these FNs and identifying the pivotal roles of their underlying hubs.

Despite the success of GNNs and Transformers in neuroimaging analysis [11, 12], accurately decoding dynamic brain states remains challenging. These models are often constrained by prohibitive computational overhead when processing high-resolution, long-sequence spatiotemporal data, and they lack the mechanistic transparency required to interpret how specific functional hubs drive these state transitions. To enhance the neurobiological interpretability of deep learning models, we propose Brain-TM, a framework that integrates a Hierarchical Transformer with the Mamba architecture [13, 14]. By efficiently capturing long-range spatiotemporal dependencies and back-projecting temporal features onto spatial attention weights, Brain-TM enables a granular analysis of latent brain states and their underlying hub topologies. Experimental results validate the model's efficacy in cognitive task decoding and reveal that global functional integration is driven by the localized activation of specific hub regions, providing a novel and interpretable perspective on functional network reconfiguration under complex brain states. In summary, the main contributions of this work are as follows:

- We propose Brain-TM, a hierarchical spatiotemporal framework integrating Transformer and Mamba to decode brain states from functional networks.
- We identify task-specific brain states and demonstrate that functional networks exhibit unique patterns that correspond to cognitive demands.
- We reveal a hub-based integration mechanism, validated through Gini analysis and centrality metrics, confirming hubs as the functional connectome's core skeleton.

2 Method

2.1 Overview

As illustrated in Fig. 1, the proposed Brain-TM framework is designed to analyze brain functional networks. Initially, the framework constructs dynamic graph embeddings from fMRI time series using a sliding window strategy and a Graph Isomorphism Network (GIN). Subsequently, the Hierarchical Spatial Block (Fig. 1.A(1)) maps brain regions to functional networks in two stages: first, it aggregates node embeddings into network representations via masked Cross-Attention; second, it models inter-network dependencies using Multi-Head Self-Attention (MHSA). Following this, the Selective Temporal Block (Fig. 1.A(2)) captures

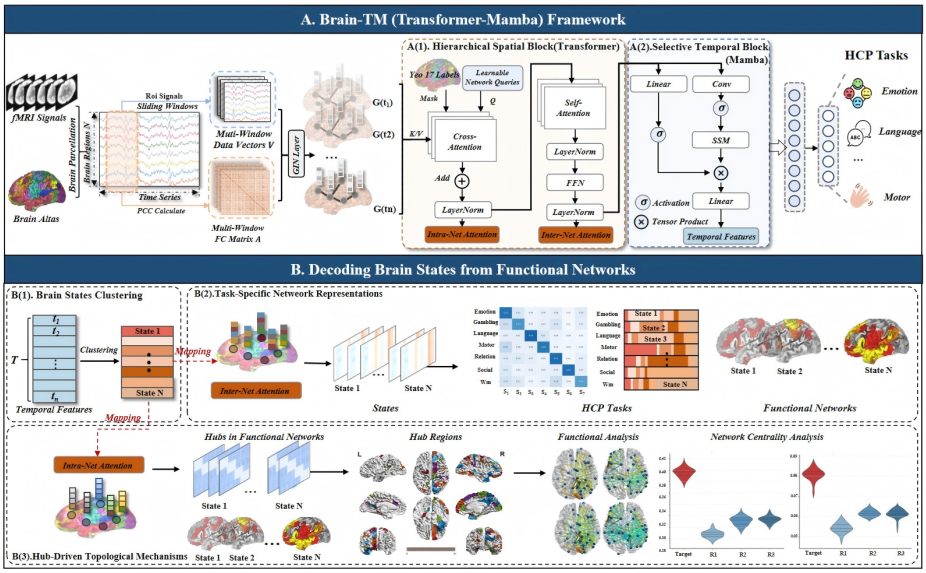

Fig. 1. The proposed architecture consists of two modules: A. The Brain-TM Framework, comprising A.(1) Hierarchical Transformer and A.(2) Mamba Block; and B. Analysis of Brain Functional Networks in Brain States, covering B.(1) Clustering, B.(2) Task-Specific Network Representations, B.(3) Hub-Based Topological Mechanisms.

the temporal evolution of these features through a Selective State Space Model (SSM), effectively integrating long-range dependencies to generate robust temporal features. Finally, as shown in Fig. 1. B, we perform a comprehensive interpretability analysis at three levels: (1) Brain States Clustering identifies latent states from the extracted temporal features to discover recurrent brain activity patterns; (2) Task-Specific Network Representations map these states back to Inter-Net Attention weights to decode task-related functional expressions; and (3) Hub-Based Topological Mechanisms integrate Intra-Net Attention to pinpoint key hub regions, subsequently validating their topological importance via network centrality benchmarking.

2.2 Brain-TM Framework

Data Preprocess: To define the functional nodes of the brain network, we employed the Schaefer parcellation [15]. The cerebral cortex was partitioned into 200 Regions of Interest (ROIs), hierarchically organized according to the Yeo 17-network functional system [7]. For each subject and task, voxel-wise BOLD signals were averaged within each ROI to generate region-wise time series. To capture the temporal dynamics of brain function, we constructed dynamic functional connectivity (dFC) matrices using a sliding window strategy [2]. Specifically, the time series were segmented into overlapping windows, and Pearson

correlation coefficients were computed between all ROI pairs within each window. These time-varying correlation matrices served as the dynamic adjacency inputs for the proposed model.

Graph Generation: We construct the dynamic brain network $G_t = (V, A_t)$, where V comprises 200 nodes defined by the Schaefer parcellation [15]. We define the adjacency matrix A_t as the sparse dynamic functional connectivity matrix, computed by thresholding Pearson correlations of BOLD signals within sliding windows. To capture the local topological heterogeneity within the dynamic brain networks, we employ a GIN variant [16]. Node features are projected into an embedding space and iteratively updated by aggregating neighbor information defined by A_t. The update rule for node v at layer l is formulated as:

$$h_{v,t}^{(l)} = \mathrm{MLP}^{(l)}\left(\sum_{u\in\mathcal{V}} A_{vu,t} h_{u,t}^{(l-1)} + \epsilon^{(l)} h_{v,t}^{(l-1)}\right) \tag{1}$$

where $h_{v,t}^{(l)}$ denotes the node embedding and $A_{vu,t} \in \{0, 1\}$ represents the binary connectivity. The learnable scalar $\epsilon^{(l)}$ adjusts the importance of the node's own features, while $\mathrm{MLP}^{(l)}$ maps the aggregated signals to deep representations $H_t^{(L)}$ for subsequent network feature extraction.

Hierarchical Spatial Module: We propose a hierarchical mechanism to obtain network level features from node level features, thereby establishing a mapping from brain regions to functional networks. The process consists of two stages: node-to-network aggregation and inter-network interaction. In the first stage, we aggregate the node embeddings $H_t^{(L)}$ into $K = 17$ functional networks representations via Cross-Attention [17]. We initialize learnable queries $Q_{net} \in R^{K\times d}$ corresponding to the functional networks. To strictly align the aggregation with the defined functional atlas, we incorporate a structural mask $M \in R^{K\times N}$. We set $M_{ij} = 0$ if region j belongs to network i, and $-\infty$ otherwise. This constraint ensures that each network representation is derived exclusively from its constituent regions. The network-level feature H_t^{intra} is computed as:

$$H_t^{intra} = \mathrm{LN}\left(\mathrm{Softmax}\left(\frac{Q(H_t^{(L)})^T}{\sqrt{d}} + M\right) H_t^{(L)} + Q\right) \tag{2}$$

where the attention weights generated in this step correspond to the Intra-Net Attention, reflecting the contribution of specific regions to their functional networks. In the second stage, to model the dependencies among these functional networks, we apply a MHSA on H_t^{intra} [17]. This will generate a representation H_t^{inter} of the network layer:

$$H_t^{inter} = \mathrm{FFN}\left(\mathrm{LN}\left(\mathrm{MHSA}(H_t^{intra}) + H_t^{intra}\right)\right) \tag{3}$$

where the attention of network connectivity corresponds to the Inter-Net Attention. H_t^{inter} is then flattened for subsequent temporal modeling.

Selective Temporal Module: To capture the temporal evolution of brain activity and identify brain states, we employ SSM based on the Mamba architecture [13, 14]. The network features H_t^{inter} are flattened and arranged into a

temporal sequence $X = \{x_1, \dots x_T\} \in \mathbb{R}^{T \times D}$ as input. The latent progression is discretized via Zero-Order Hold into the recursive rule:

$$h_t = \overline{\mathbf{A}}_t h_{t-1} + \overline{\mathbf{B}}_t x_t, \quad y_t = \mathbf{C}_t h_t \tag{4}$$

where $h_t \in \mathbb{R}^N$ is the latent hidden state and $\mathbf{C}_t \in \mathbb{R}^{D \times N}$ is the output projection matrix. The discrete transition parameters $\overline{\mathbf{A}}_t = \exp(\Delta_t \mathbf{A})$ and $\overline{\mathbf{B}}_t = (\Delta_t \mathbf{A})^{-1}(\exp(\Delta_t \mathbf{A}) - \mathbf{I}) \cdot \Delta_t \mathbf{B}_t$. Unlike Linear Time-Invariant systems, we implement an input-dependent selection mechanism where Δt, B_t and C_t are functions of x_t, the generated output sequence $Y = \{y_1, \dots y_T\}$ encapsulates temporal features for model classification and subsequent brain state recognition.

2.3 Decoding Brain States from Functional Networks

To interpret the spatiotemporal features learned by Brain-TM, we propose a hierarchical analysis approach to decode brain states from dynamic functional networks. First, we identify latent brain states through feature clustering and map these states back to spatial attention weights to analyze functional networks expressions across different cognitive tasks. Secondly, we employ Gini analysis to identify Distributed and Hub-Based patterns. We calculate Network and Region Gini indices to evaluate global segregation and internal network expression. Finally, we investigate the topological characteristics of functional hubs using centrality and connectivity strength, benchmarking them against random sets across all time windows to establish significance.

3 Experiment and Results

3.1 Experimental Settings and Performance.

Experimental Settings. We evaluated Brain-TM using task-fMRI data from the HCP dataset [18], covering seven cognitive domains (7 tasks) preprocessed via standard pipelines [19]. Performance was assessed using Accuracy (ACC), F1 Score, and AUC via subject-level stratified 5-fold cross-validation, where all windows from one subject are fully assigned to either training or test splits to eliminate data leakage. The model was implemented in PyTorch and optimized via Adam (100 epochs, batch size 32, learning rate 0.0005). To determine optimal temporal granularity, we performed sensitivity analysis across sliding window sizes of [10, 15, 20, 25, 30, 35] TRs.

Table 1. Performance comparison of different methods on three metrics (Unit: %).

Method	GAT	GCN	BrainNetCNN	GraphSAGE	GIN	BrainGNN	**Brain-TM**
ACC(%)	78.60 ± 10.45	91.20 ± 1.70	90.60 ± 4.04	92.40 ± 2.20	93.87 ± 0.66	94.40 ± 4.04	**94.71 ± 1.27**
AUC(%)	-	93.70 ± 2.60	-	95.30 ± 1.60	-	-	**99.50 ± 0.20**
F1(%)	77.00 ± 11.58	-	90.96 ± 3.50	-	-	94.34 ± 3.27	**94.71 ± 1.28**

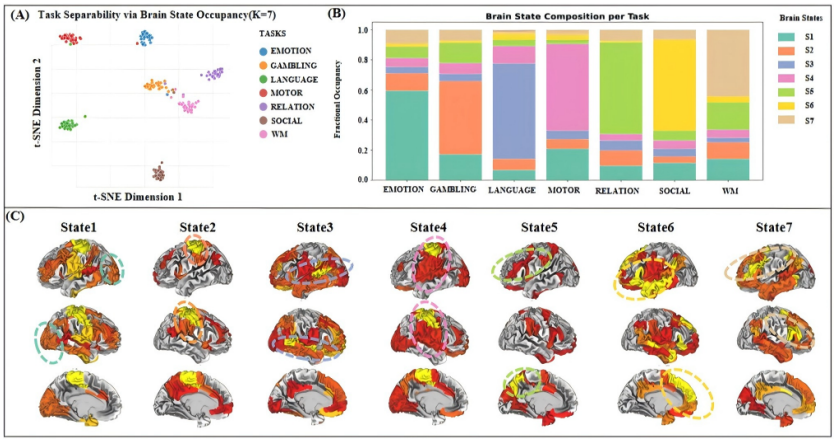

Fig. 2. Representations of functional networks in brain states. (A) t-SNE visualization. (B) Task-state statistical distribution. (C) Functional networks activation patterns.

Experimental Performance. To demonstrate the effectiveness of Brain-TM, we compared it with 6 baselines, categorizing them into general GNNs (GAT [20], GraphSAGE [21], GCN[22], GIN[16]) and brain-specific models (BrainNetCNN [23], BrainGNN[24]). Table 1 reports the average performance metrics (ACC, AUC and F1) obtained from 5-fold cross-validation in 6 window sizes. As shown in Table 1, Brain-TM achieved state-of-the-art performance with an ACC of 94.71% and an AUC of 99.50%. It is superior to baselines such as GAT (78.60%) and BrainNetCNN (90.60%), while also surpassing GIN (93.87%) and BrainGNN (94.40%). Brain-TM's integration of the Hierarchical Transformer for network interactions and the Mamba Module for long-range temporal dynamics results in superior classification capability.

3.2 The Analysis of Brain States from Functional Networks

Task-Specific Network Representations in Brain States Our results demonstrate that brain states manifest as specific functional network patterns that strictly correspond to distinct cognitive tasks. We screened $K = 1$–15 via Silhouette Score and elbow inertia curve[25], where metrics peaked at $K = 7$ for optimal clustering, and further validated the seven identified latent states with t-SNE (Fig. 2.(A)) to reveal distinct, task-specific clusters. Each task is dominated by a unique state, highlighting the high task-specificity of these dynamic brain states(Fig. 2.(B)). Specifically, Fig. 2.(C) reveals that short windows favor Somatomotor and Control networks (aligning States 4/7 with MOTOR/WM), while medium-to-long windows highlight Default, Attention, and Limbic networks (aligning States 3/6 with SOCIAL/LANGUAGE), and SalVentAttn, Cont, and VisCent networks (aligning State 2/5/1 with GAMBLING/RELATIONAL/EMOTION) [26].

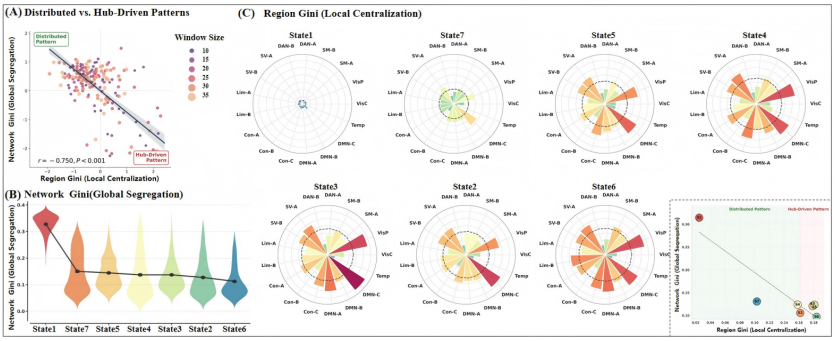

Fig. 3. Hub-Based network mechanisms. (A) Distributed and Hub-Based patterns. (B)Network Gini(Global Segregation). (C) Region Gini(Local Centralization).

Hub-Based Mechanisms Across Brain States Furthermore, our analysis reveals that the expression of brain functional networks across brain states is primarily driven by the dominant role of internal hub nodes. We quantified nodal activation inequality using Gini coefficient analysis across all windows, identifying two distinct activation patterns: a Distributed Pattern (low Gini) and a Hub-Based Pattern (high Gini) (Fig. 3.(A)). At the global level, Network Gini indices vary across brain states, with states such as S2, S3, and S6 exhibiting relatively lower global segregation (Fig. 3.(B)). However, at the regional level, these same states show a significant increase in Region Gini coefficients within the default mode, control, salience, and peripheral visual systems (Fig. 3.(C)). This indicates that while global network activation appears distributed, internal network expression is dominated by localized hub activation. Biologically, these hub patterns align with DMN-mediated connectivity, Salience/Control-driven state switching [27–29], and hierarchical visual processing. In summary, the dynamic expression of brain functional networks across varying cognitive states is fundamentally driven by the dominant role of their internal hub nodes.

Topological Characteristics of Functional Hubs Finally, our results confirm that hub nodes occupy a dominant position in integrating whole-brain dynamic functional networks. We validated this core role by analyzing the top 51 highest-weighted nodes. First, spatial overlap analysis (Fig.4.(A)) confirms that these hubs (blue regions) align with global high-weight vertices, constituting the functional connectome's core skeleton. Second, topological reconstruction (Fig.4.(B)) reveals that hubs retain a dense, integrated sub-network, contrasting with the sparse connectivity of random groups. Finally, quantitative results (Fig.4.(C)) demonstrates superior Degree, Eigenvector, and Betweenness Centrality[30] with lower temporal volatility than random baselines.

3.3 Ablation Study

To validate the contribution of GIN, Hierarchical Transformer, and Mamba, we conducted an ablation study (Table 2). We performed a full grid search for the

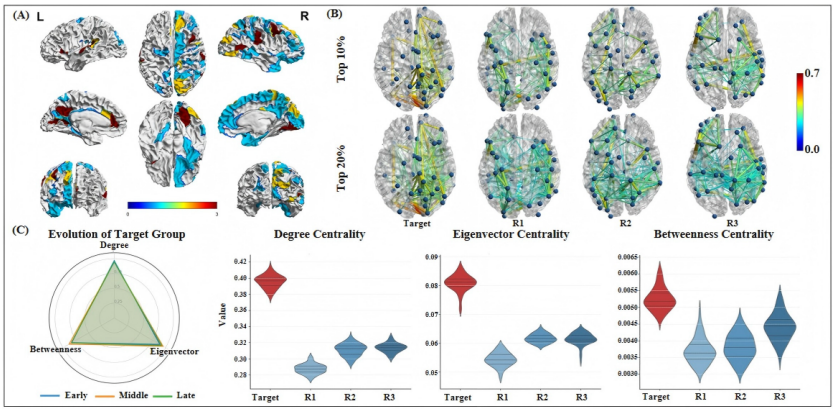

Fig. 4. Topological characteristics of functional hubs. (A) Spatial overlap analysis. (B) Sub-network topology reconstruction. (C) Centrality benchmark comparisons.

standalone Temporal Transformer baseline (learning rate: 10^{-4}–10^{-3}, dropout rate: 0.1–0.5) to guarantee a fair experimental comparison. Replacing the Mamba module with a standard Temporal Transformer caused substantial performance degradation (ACC 82.72%) and increased training time (135.14±44.09s), underscoring Mamba's efficiency in capturing long-range dependencies without quadratic bottlenecks. Excluding the GIN module decreased ACC to 91.24%, confirming its necessity for initial topological embeddings. Removing the Hierarchical Transformer lowered ACC to 93.73% and unexpectedly increased computational time (130.85±65.69s). This occurs because omitting the spatial aggregation (from 200 ROIs to 17 networks) passes massive uncompressed dimensions directly to the temporal module. The full Brain-TM framework achieves the best ACC and F1 alongside optimal stability (100.48±13.55s), confirming that the synergistic integration of these modules is optimal for brain network analysis.

Table 2. Ablation study of different components in Brain-TM on the HCP dataset.

GIN	Transformer	Mamba	ACC (%)	F1 (%)	AUC (%)	Time (s/ep.)
×	✓	✓	91.24	91.24	98.03	57.64 ± 35.08
✓	×	✓	93.73	93.71	**99.61**	130.85 ± 65.69
✓	✓	×	82.72	82.74	97.53	135.14 ± 44.09
✓	✓	✓	**94.71**	**94.71**	99.50	**100.48 ± 13.55**

4 Conclusion

In this study, we propose Brain-TM, a hierarchical spatiotemporal framework to decode brain states from functional networks. By capturing spatiotemporal dependencies and back-projecting temporal features onto spatial attention weights,

Brain-TM identifies task-specific network representations, confirming that latent brain states align with distinct cognitive tasks. Our analysis uncovers a hub-based mechanism across brain states, where global integration is orchestrated by localized hub activations. Furthermore, the topological characteristics of functional hubs are rigorously validated through centrality analysis. Future work will test additional datasets for broader generalizability. In summary, Brain-TM provides a novel and interpretable perspective for understanding the roles of functional networks in characterizing brain states.

Acknowledgments. This work was supported by the National Natural Science Foundation of China (62376219); the Fundamental Research Funds for the Central Universities (G2026KY07010).

Disclosure of Interests. The authors have no competing interests to declare that are relevant to the content of this article.

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