

Multilayer Modularity-Aware Graph Autoencoder for Detecting Subpopulation Community Structure in Dynamic Brain Networks

Kai-Jun See¹, Fuad Noman¹, Raphaël C.-W. Phan¹, Hernando Ombao²,
and Chee-Ming Ting¹

¹ School of Information Technology, Monash University Malaysia
{kai.jun.see, fuad.noman, raphael.phan, ting.cheeming}@monash.edu

² Statistics Program, King Abdullah University of Science and Technology (KAUST)
hernando.ombao@kaust.edu.sa

Abstract. Deciphering dynamic brain states from functional magnetic resonance imaging (fMRI) requires disentangling temporal network fluctuations from intrinsic subject-level heterogeneity. However, most existing graph learning methods assume an individual-based or homogeneous population, failing to account for latent subject subpopulations that exhibit distinct node-level community structures. To address this, we propose a Multilayer Modularity-aware Graph Autoencoder (MMGAE) utilizing a hierarchical two-stage approach. First, we identify latent subpopulations by clustering Weighted Stochastic Block Model (WSBM) parameters derived from shared prior node communities. Second, these subpopulation labels guide a novel contrastive coupling mechanism within the MMGAE. This mechanism enforces community-constrained edges to preserve local node topology (modular organization) while utilizing a contrastive coupling objective to explicitly differentiate between disparate subject subgroups across network layers. The resulting community partition from each modularity-aware subject embedding is subsequently integrated into a Markov-switching WSBM to identify time-resolved brain states. This pipeline effectively uncovers the specific modular organization defining each subpopulation before analyzing temporal dynamics. We validated the framework on Human Connectome Project task fMRI data. The MMGAE achieved superior consensus clustering performance compared to baseline methods, validating its ability to resolve subpopulation-specific patterns. Furthermore, the model shows significant improvement in identifying distinct brain states characterized by varying levels of network segregation and integration between subgroups. The code is available at <https://github.com/KaiJunSee/MMGAE>.

Keywords: Community detection · Deep graph clustering · Dynamic functional connectivity · Multi-subject network · Multilayer modularity.

1 Introduction

Characterizing the dynamic organization of functional brain networks is essential for understanding neural mechanisms and cognitive processes [13,26]. Functional

magnetic resonance imaging (fMRI) allows researchers to map these macroscopic networks by representing the brain as a complex graph [17,23]. Within this framework, community detection has emerged as a powerful analytical tool for the identification of highly interconnected groups of brain regions (nodes) that share functional specialization [7,22,28]. However, brain network topology is not static and it constantly reconfigures, transitioning through various dynamic states during task performance and rest [3,5,18,27].

To capture these temporal dynamics, multilayer network approaches, such as multilayer modularity maximization [1,19], have been developed to track evolving node-level community structures across time. While effective, most existing dynamic methods focus primarily on single-subject analysis [4] or assume a completely homogeneous population, attempting to uncover a single, common community partition across all individuals [6,29]. Similarly, recent deep graph learning models for brain networks largely overlook inter-subject variability [2,15,16,21]. These conventional approaches fundamentally fail to account for the presence of latent subject subpopulations, distinct groups of individuals who exhibit fundamentally different underlying baseline network topologies [9,10].

To address this methodological gap, we propose a unified framework integrating Multilayer Modularity-aware Graph Autoencoder and Weighted Stochastic Block Model (MMGAE-WSBM) to explicitly disentangle subject-level heterogeneity in the community structures from temporal brain dynamics. Rather than enforcing a universal group average, our approach introduces a hierarchical two-stage strategy. First, we identify latent subject subpopulations by clustering WSBM parameters [6,10] derived from shared prior node communities. Second, we leverage these subpopulation labels to guide a novel contrastive coupling mechanism within the supra node similarity matrix. This mechanism enforces community-constrained edges to preserve local node modularity while simultaneously maximizing the separability of different subgroups in the embedding space. The resulting modularity-aware embedding is then integrated into a Markov-switching WSBM [25] to identify time-resolved brain states.

Our contributions are threefold: 1.) A novel multilayer graph learning framework that explicitly disentangles subject-level heterogeneity from temporal brain dynamics. 2.) Integration of latent subject subpopulations to guide a novel contrastive coupling mechanism, preserving local node-level community structure. 3.) A state identification pipeline utilizing a Markov-switching WSBM to uncover distinct, subpopulation-specific dynamic brain motifs.

2 Methods

Fig. 1 shows an overview of the MMGAE-WSBM for detecting subpopulation and dynamic community structure in subject- and time-varying brain networks.

2.1 Multi-Subject Time-Varying Brain Networks

We denote a set of undirected graphs in subject- and time-varying fMRI functional brain networks as $\mathcal{G} = \{G_{rt}\}_{r=1,\dots,R;t=1,\dots,T}$ that share a set of N nodes

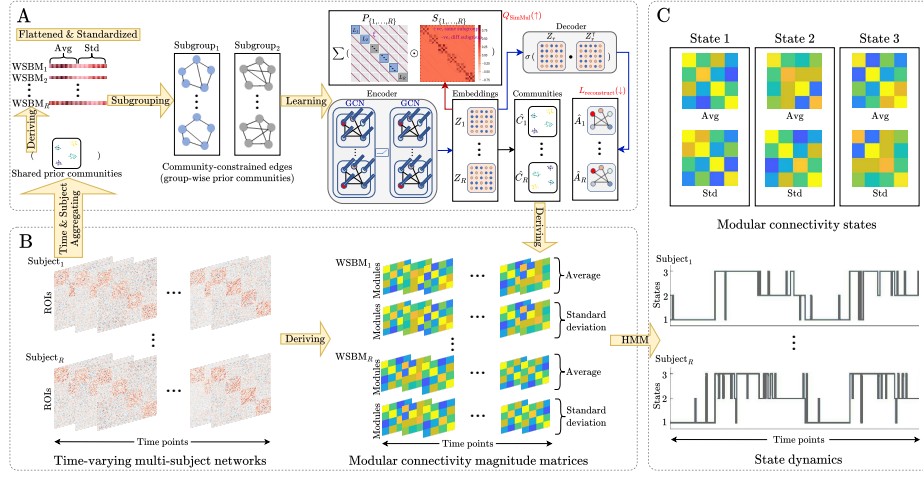


Fig. 1. Architecture of MMGAE-WSBM framework, which consists of three parts: (A) Community detection via MMGAE with contrastive coupling for different identified subgroups, (B) Derivation of time-resolved community connectivity magnitudes' average and standard deviation into WSBMs, (C) Dynamic modular connectivity state identification via hidden Markov modeling.

$V = \{v_i\}_{i=1,\dots,N}$ (brain regions of interest (ROIs)) for a group of R subjects in T sliding time windows. Each rt -th graph $G_{rt} = (V, E_{rt}, X_{rt})$ represents the network for r -th subject and t -th window, with a set of connectivity edges $E_{rt} = \{e_{ijrt}\}$ where e_{ijrt} is the edge between a pair of nodes v_i and v_j . We have a node attribute matrix $X_{rt} = [x_{1rt}, \dots, x_{Nrt}]^T \in \mathbb{R}^{N \times M}$ for graph G_{rt} where $x_{irt} \in \mathbb{R}^M$ is the real-value attribute vector for node v_i . The topological structure of graph G_{rt} can be represented by an adjacency matrix $A_{rt} = [a_{ijrt}] \in \{0, 1\}^{N \times N}$ where $a_{ijrt} = 1$ if there is a connecting edge $e_{ijrt} \in E_{rt}$ between nodes v_i and v_j , else $a_{ijrt} = 0$. We suppose no self-connection, i.e., $a_{iirt} = 0$.

2.2 Initial Community Detection and Subgrouping

For each subject r and time window t , the functional connectivity (FC) is computed based on Pearson correlations of fMRI time series between pairs of ROIs. We apply FC as the node attribute X_{rt} to represent the statistical dependence between nodes. After time aggregation, we obtain the time-averaged FC, $X_r = \frac{1}{T} \sum_{t=1}^T X_{rt}$ for each subject, and perform a proportional thresholding [12] function $\phi(\cdot)$ to obtain the adjacency matrix $A_r = \phi(X_r)$ with fixed density of edges (strongest connections with largest absolute correlation coefficients) across all subjects for exploring meaningful graph topology in multi-subject community detection. Then the average FC over subjects, $X = \frac{1}{R} \sum_{r=1}^R X_r$ and consensus adjacency matrix $A = \phi(\sum_{r=1}^R [(D_r + I_N)^{-\frac{1}{2}} (A_r + I_N) (D_r + I_N)^{-\frac{1}{2}}])$ are computed where I_N is $N \times N$ identity matrix added for self-connections and D_r is diagonal

degree matrix of A_r . A incorporates network structure information aggregated across all subjects.

For initial shared prior community detection, we perform spectral clustering [20] on the weighted consensus adjacency matrix $W = A \odot |X|$. Spectral clustering is used for its ability to effectively cluster data points with complex, non-convex shapes, and to detect the optimal number of communities using the eigenvalue gap heuristic. With the overall shared prior communities, the WSBM parameters of average and standard deviation (based on the magnitude of $|X_r|$) are computed for each subject, see Subsection 2.4. Then the subgroups are obtained by clustering WSBM parameters, and the optimal number of subgroups is selected empirically based on the best state identification performance. The prior community detection step is now repeated for each subgroup to obtain subpopulation communities. To enforce modularity-preserving node topology, new adjacency matrices $\{A_r\}_{r=1,\dots,R}$ are constructed from community edges A_c when $a_{ijc} = 1$ if nodes v_i and v_j belong to same community, where $A_r = \phi(A_c \odot X_r)$. This operation acts as an informed structural regularizer to only retain edges that are both statistically strong in the subject’s data (X_r) and consistent with the subgroup’s modular organization (A_c), effectively filtering idiosyncratic noise.

2.3 Multilayer Modularity-Aware Graph Autoencoder

Graph Autoencoder. In Fig. 1 (A), the graph autoencoder (GAE) aims to learn graph embeddings $\{Z_r\}_{r=1,\dots,R}$ and capture the topological information across subjects. We apply a two-layered graph convolutional network (GCN) to encode, for subject r , the graph data G_r into the graph embedding $Z_r \in \mathbb{R}^{N \times F}$, i.e., $F \ll M$. We then apply an edge prediction layer on the inner product of Z_r to decode and reconstruct the adjacency matrix $\hat{A}_r = \sigma(Z_r Z_r^\top)$ where $\sigma(\cdot)$ is sigmoid function. The reconstruction loss between actual and reconstructed adjacency matrices, A_r and $\hat{A}_r$ for each subject is computed based on the binary cross-entropy $L_r = -\frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N [a_{ijr} \log(\hat{a}_{ijr}) + (1 - a_{ijr}) \log(1 - \hat{a}_{ijr})]$. The total reconstruction loss $L_{\text{reconstruct}} = \sum_r L_r$ is minimized in training so that the latent embeddings retain much of the crucial information.

Supra Community-based Modularity Matrix. Supra community-based modularity matrix P is constructed based on the multilayer modularity [19]:

$$Q_{\text{multilayer}} = \frac{1}{2\mu} \sum_{ijrs} [(A_{ijr} - \gamma_r \frac{d_{ir}d_{jr}}{2m_r})\delta_{rs} + \delta_{ij}\xi_{jrs}]\delta(k_{ir}, k_{js}) \quad (1)$$

where k_{ir} is the community assignment of node v_i in layer r , $\delta(k_{ir}, k_{js}) = 1$ if nodes v_i and v_j belong to the same community, and 0 otherwise. Here, we set homogeneity that the same node v_j across different subjects belongs to the same community, i.e., $\delta(k_{jr}, k_{js}) = 1$ and leave subgroup-wise heterogeneity to the next subsection (Supra Contrastive Node Similarity Matrix). ξ_{jrs} is coupling parameter between layer r and s of the same nodes v_j (because δ_{ij} enforces

$v_i = v_j$), smaller ξ detects less similar communities across layers. $d_{ir} = \sum_j a_{ijr}$ is the degree of node v_i , $2m_r = \sum_i d_{ir}$ is total number of edges in layer r , γ_r is resolution parameter to control number of communities (more communities with larger γ). $2\mu = \sum_{js}(d_{js} + \xi_{js})$ is total number of edges within and across layers.

We construct the supra community-based modularity matrix $P = P_{i'j'} \in \mathbb{R}^{NR \times NR}$ including all R subjects, where $P_{i'j'} = (A_{ijr} - \gamma_r \frac{d_{ir}d_{jr}}{2m_r})\delta_{rs}$ within same layer (subject) r along the diagonal, $P_{i'j'} = \delta_{ij}\xi_{jrs}$ for same nodes v_j across different layers, and $P_{i'j'} = 0$ otherwise.

Supra Contrastive Node Similarity Matrix. To learn modular embeddings across layers, we generalize the single-layer modularity-aware GAE (MGAE) [24] for similarity-based multilayer modularity Q_{SimMul} , by adding a group term $\delta(g_r, g_s)$ and modifying the $\delta(k_{ir}, k_{js})$ term in (1) to an exponential term that measures node similarities (to ease the latter K-means clustering on embeddings for communities):

$$Q_{\text{SimMul}} = \frac{1}{2\mu} \sum_{ijrs} [(A_{ijr} - \gamma_r \frac{d_{ir}d_{jr}}{2m_r})\delta_{rs} + \delta_{ij}\xi_{jrs}] \odot \delta(g_r, g_s) e^{-\eta \|z_{ir} - z_{js}\|_2^2} \quad (2)$$

where $\delta(g_r, g_s) = 1$ if layers r and s belong to the same group, and -1 otherwise, forming contrastive coupling at the subgroup level to explicitly differentiate between disparate subgroups across network layers in embedding space. The exponential term acts as a soft counterpart of the common community indicator $\delta(k_{ir}, k_{js})$, the higher its value, the closer the node v_{ir} and v_{js} in the embedding space. η serves as a regulating parameter to the magnitude of $\|z_{ir} - z_{js}\|_2^2$.

This exponential term can also be defined as supra node similarity matrix $S = S_{i'j'} \in \mathbb{R}^{NR \times NR}$ including all R subjects, where $S_{i'j'} = e^{-\eta \|z_{ir} - z_{jr}\|_2^2}$ within same layer (subject) r along the diagonal. Through $\delta(g_r, g_s)$, we set heterogeneity between subgroups that $S_{i'j'} = -e^{-\eta \|z_{jr} - z_{js}\|_2^2}$ for same nodes v_j across subjects from different subgroups, and $S_{i'j'} = e^{-\eta \|z_{jr} - z_{js}\|_2^2}$ within same subgroups.

Objective Function. Hence, $Q_{\text{SimMul}} = \frac{1}{2\mu} \sum_{i'j'} (P_{i'j'} \odot S_{i'j'})$ where $\odot$ is element-wise multiplication. We have modularity-maximized structural information from $P_{i'j'}$ and closer-distance attribute information from $S_{i'j'}$ for embedding learning across network layers.

The overall loss L_{overall} is computed as the total objective function (minimizing reconstruction loss and maximizing similarity-based multilayer modularity): $L_{\text{overall}} = L_{\text{reconstruct}} - \beta Q_{\text{SimMul}}$ where β is the balancing parameter between both losses.

The obtained embeddings are performed K-means clustering for node clustering/community assignment vectors $\hat{C}_r \in \{1, \dots, K\}^N$ across subjects.

2.4 Markov-Switching WSBM for Dynamic State Identification

In Fig. 1 (B), we compute weighted stochastic block models (WSBMs) for 2 measures: average $\Theta_\mu \in \mathbb{R}^{K \times K}$ and standard deviation $\Theta_\sigma \in \mathbb{R}^{K \times K}$ based on the FC

matrix per subject and time, where each block accounts for the central tendency (average) and dispersion (standard deviation) of community connectivity values. We utilize hidden Markov model (HMM) for the time-resolved WSBMs, suitable for sequential data and being efficient computationally due to small number of parameters. This is augmenting the multi-slice WSBMs across time windows with a Markov-switching model for temporal dynamics, called MS-WSBM. Our hierarchical architecture maintains informational independence between parts. Part A discovers subgroups using time-averaged parameters (global profiles), whereas Part B utilizes transient windowed dynamics for state identification.

3 Experiments and Results

3.1 Experimental Setup

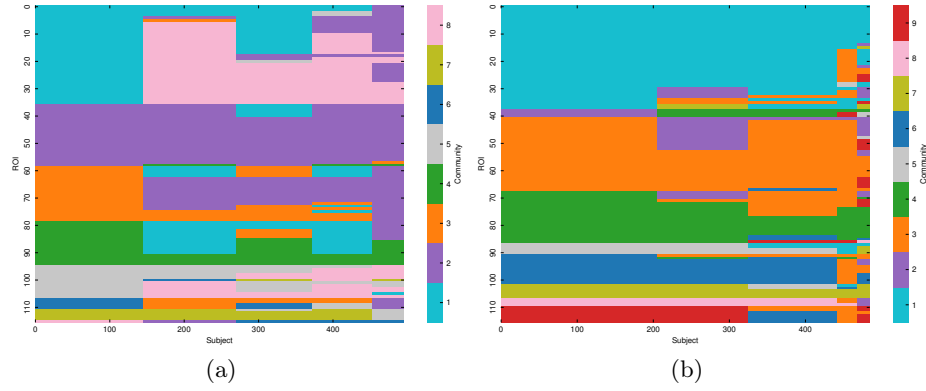
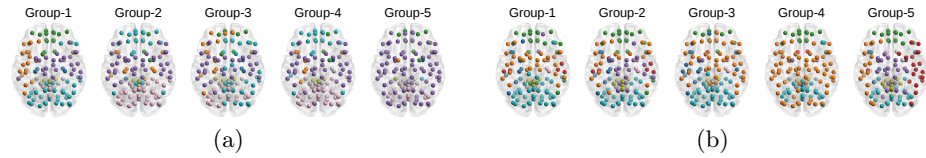
1. Dataset: We apply the proposed MMGAE-WSBM framework to task fMRI data from Human Connectome Project (HCP) [30] on motor ($R = 496$ subjects, $T = 250$ time windows) and language ($R = 485$ subjects, $T = 295$ time windows) tasks. The data were minimally preprocessed with HCP preprocessing pipelines version of v3.13.2 [8]. We parcellate the brain into $N = 116$ ROIs with automated anatomical labeling (AAL) and compute ROI-wise fMRI time series over sliding windows of 30 time points (step size = 1 TR).
2. Training: The proposed model operates as an unsupervised, transductive learning framework. We train MMGAE using Adam optimizer (lr = 0.001, wd = 1e-3) over 200 epochs. Hyperparameters ($\gamma = 1$, $\xi = 1$, $\eta = 1$, $\beta = 1$) were empirically tuned by monitoring objective loss convergence and maximizing cluster consensus. We observed the model to be robust to variations.
3. Evaluation: In multi-subject community detection, consensus clustering is combining multiple partitions of the same population network into a single, robust consensus partition $\hat{C}$ which is then compared with $\hat{C}_r$ across subjects within the same group. Performance metrics include adjusted mutual information (AMI), adjusted Rand index (ARI), accuracy (ACC), F1-score (F1). In dynamic state identification, comparison of estimated state time courses across subjects with the experimental ground truth is assessed using Rand index (RI), ACC, F1. To ensure stability, we utilized K-means++ initialization with 20 replicates to approximate global optima for each subject.
4. Benchmarking: For fair benchmarking, baseline methods were rigorously tuned following their publicly available implementations, ensuring that all models were trained and evaluated under identical computational conditions.

3.2 Cluster Consensus Results

Table 1 reports intra-group cluster consensus, not a comparison against external biological ground-truth labels. The proposed MMGAE has performed the best among methods. The 1.0 scores demonstrate that the contrastive coupling mechanism ($\delta(g_r, g_s)$) in (2) successfully minimizes intra-group variance, mathematically forcing the individual embeddings in each subgroup to converge into

Table 1. Cluster consensus results of graph clustering methods over subject groups for motor and language task experiments.

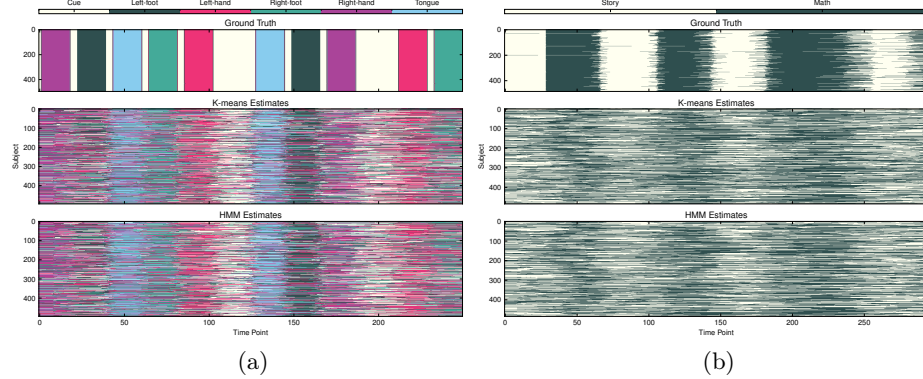
Task	Method	AMI	ARI	ACC	F1
Motor	Spectral [20]	0.1541 ± 0.0917	0.1178 ± 0.0941	0.4566 ± 0.1050	0.2978 ± 0.0883
	MGAE [24]	0.2318 ± 0.0617	0.1625 ± 0.0583	0.4114 ± 0.0600	0.3418 ± 0.0614
	GenLouvain [14]	0.7421 ± 0.0679	0.7762 ± 0.0893	0.9028 ± 0.0662	0.8803 ± 0.1107
	MMGAE (Ours)	1.0000 ± 0.0000	1.0000 ± 0.0000	1.0000 ± 0.0000	1.0000 ± 0.0000
Lang.	Spectral [20]	0.1699 ± 0.0863	0.1024 ± 0.0703	0.3978 ± 0.0740	0.3011 ± 0.0914
	MGAE [24]	0.2286 ± 0.0713	0.1562 ± 0.0635	0.3994 ± 0.0643	0.3310 ± 0.0641
	GenLouvain [14]	0.7709 ± 0.1243	0.7944 ± 0.1334	0.9196 ± 0.0947	0.9180 ± 0.1040
	MMGAE (Ours)	1.0000 ± 0.0000	1.0000 ± 0.0000	1.0000 ± 0.0000	1.0000 ± 0.0000

**Fig. 2.** Brain community partitions detected by MMGAE across subjects from (a) motor and (b) language task fMRI, given 5 hidden subject groups each identified as prior. The brain ROIs were color-coded and sorted by assigned communities.**Fig. 3.** Connectome plots of subpopulation community partitions detected by MMGAE over (a) motor and (b) language tasks. ROIs are colored by assigned communities.

a stable, coherent representation (as shown in Fig. 2). Aggregating from varied subsample data creates a consensus matrix to identify stable community structure and determine the optimal number of groups (as shown in Fig. 3), which is particularly vital in neuroimaging and complex network science. GenLouvain, as a multilayer modularity maximization method, ranks second due to the lack of customized interlayer coupling across different subgroups [11]. Other single-layer methods perform poorly as expected, because they lack data pooling across multiple layers to estimate the common community structure.

Table 2. State identification results of time series methods for task experiments.

Task	Method	Clustering	RI	ACC	F1
Motor	K-means	Spectral [20]	0.7290 $\pm$ 0.0243	0.4357 $\pm$ 0.0457	0.4385 $\pm$ 0.0495
		MGAE [24]	0.7279 $\pm$ 0.0217	0.4258 $\pm$ 0.0498	0.4266 $\pm$ 0.0548
		GenLouvain [14]	0.7242 $\pm$ 0.0185	0.3974 $\pm$ 0.0462	0.3961 $\pm$ 0.0510
		MMGAE (Ours)	0.7330$\pm$0.0247	0.4433$\pm$0.0469	0.4457$\pm$0.0512
	MS-WSBM	Spectral [20]	0.6897 $\pm$ 0.0951	0.4286 $\pm$ 0.0518	0.4190 $\pm$ 0.0716
		MGAE [24]	0.7282 $\pm$ 0.0224	0.4246 $\pm$ 0.0489	0.4246 $\pm$ 0.0548
		GenLouvain [14]	0.7238 $\pm$ 0.0203	0.3977 $\pm$ 0.0471	0.3956 $\pm$ 0.0523
		MMGAE (Ours)	0.7334$\pm$0.0258	0.4430$\pm$0.0488	0.4461$\pm$0.0525
Lang.	K-means	Spectral [20]	0.5206 $\pm$ 0.0283	0.5861 $\pm$ 0.0607	0.5627 $\pm$ 0.0719
		MGAE [24]	0.5211 $\pm$ 0.0283	0.5866 $\pm$ 0.0620	0.5695 $\pm$ 0.0692
		GenLouvain [14]	0.5206 $\pm$ 0.0279	0.5855 $\pm$ 0.0615	0.5724$\pm$0.0677
		MMGAE (Ours)	0.5216$\pm$0.0320	0.5869$\pm$0.0637	0.5673 $\pm$ 0.0730
	MS-WSBM	Spectral [20]	0.5172 $\pm$ 0.0271	0.5761 $\pm$ 0.0603	0.5330 $\pm$ 0.0915
		MGAE [24]	0.5225$\pm$0.0300	0.5894$\pm$0.0638	0.5747 $\pm$ 0.0701
		GenLouvain [14]	0.5219 $\pm$ 0.0296	0.5890 $\pm$ 0.0621	0.5788$\pm$0.0668
		MMGAE (Ours)	0.5225 $\pm$ 0.0335	0.5885 $\pm$ 0.0650	0.5706 $\pm$ 0.0738

**Fig. 4.** Regime change tracking in the MMGAE-derived community connectivity measures of brain networks across subjects from (a) motor and (b) language task fMRI with 6 and 2 different states respectively. (Top) Ground truth task state time courses. (Middle & Bottom) Dynamic state estimates by K-means clustering and MS-WSBM.

3.3 State Identification Results

In Table 2, the cluster partitions from proposed MMGAE have performed overall the best in terms of state identification, especially in motor task. While the improvements in metrics may appear numerically modest due to expected biological noise and asynchrony in dynamic states, the consistent performance advantage of MMGAE-WSBM over baseline methods across a large cohort ($R = 496$ for motor, $R = 485$ for language) demonstrates stable methodological gains. This evaluation serves as a rigorous proof of concept validating the proposed framework’s ability to disentangle subject-level heterogeneity from noisy fMRI-based

temporal dynamics for state identification. While the single-layer MGAE performs better in language task, this may be due to unsynchronized states across subjects (as shown in Fig. 4 (b)), which creates challenges for multilayer methods when partitions are more likely to be inconsistent.

4 Conclusion

We developed the MMGAE-WSBM to decipher dynamic brain states while explicitly accounting for subject-level heterogeneity. Our hierarchical approach first discovers latent subpopulations using WSBMs, which then guide a novel contrastive coupling mechanism in MMGAE. This successfully disentangles inter-subject variations from local, node-level community structure. Validation on HCP task fMRI data demonstrates that MMGAE achieves superior consensus clustering compared to baseline methods and significantly improves the identification of time-resolved dynamic brain states. To address the challenge of less consistent partitions in unsynchronized task states across subjects, future work will explore integrating high-performance sequence modeling architectures to better capture complex and asynchronous temporal dynamics.

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

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