Topological State-Space Estimation of Functional Human Brain Networks

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Introduction

We present a topological data analysis (TDA) approach for estimating a state space in dynamically changing functional human brain networks. The Wasserstein distance that measures the 0D and 1D topological changes in the networks is used in measuring the difference in states. The method is used in determining the very accurate heritability map of the state space directly.

Graph filtrations

Consider weighted graph $\mathcal{X} = (V, E)$ consisting of node set $V = \{1, 2, \cdots, p\}$ and edge weights $W = (W_{ij})$ between nodes i and j. We have sorted edge weight set E

$$E : \min_{j,k} W_{jk} = W_{(1)} < W_{(2)} < \cdots < W_{(q)} = \max_{j,k} W_{jk}.$$

Let $\mathcal{X}_\epsilon = (V, W_\epsilon)$ be a binary graph obtained after thresholding edge weights at ϵ with adjacency matrix W_ϵ. The *graph filtration* is the sequence of nested graphs (Fig. 1) (Das et al., 2022).

$$\mathcal{X}_{W_{(1)}} \supset \mathcal{X}_{W_{(2)}} \supset \cdots \supset \mathcal{X}_{W_{(q)}}.$$

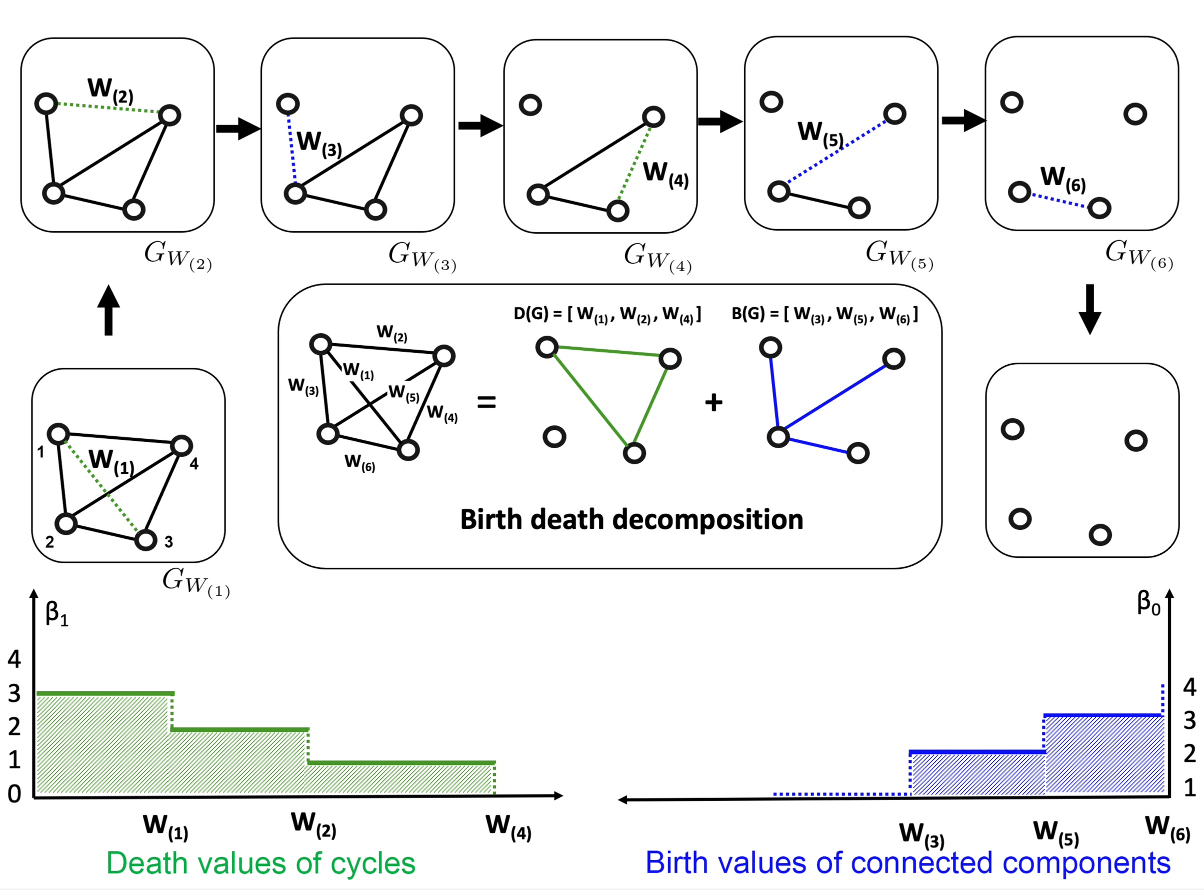

Fig. 1. Schematic of graph filtration. We order edge weights as $W_{(1)} < W_{(2)} < \cdots < W_{(6)}$. We remove each edge of the graph one at a time and construct the collection of nested graphs called the *graph filtration*. During the graph filtration, we obtain the birth set of connected components E_b and the death set E_d of cycles. Using the birth and death sets, we can compute the Betti-0 (lower right) and Betti-1 (lower left) curves characterizing topology.

Topological Embedding

During the graph filtration, connected components are born at birth values

$$E_b = \{b_{(1)}, b_{(2)}, \cdots, b_{(q_0)}\}$$

with $q_0 = p - 1$ while while cycles die at death values

$$E_d = \{d_{(1)}, d_{(2)}, \cdots, d_{(q_1)}\}$$

with $q_1 = (p-1)(p-2)/2$. Then edge weight set $E = \{W_{(1)}, \cdots, W_{(q)}\}$ has the unique decomposition called the birth-death decomposition (Fig. 1) (Songdechakraiwut and Chung, 2022)

$$E = E_b \cup E_d, \quad E_b \cap E_d = \emptyset.$$

The decomposition is used to topologically embed dynamically changing connectivity matrix into birth and death sets (Fig. 2-right).

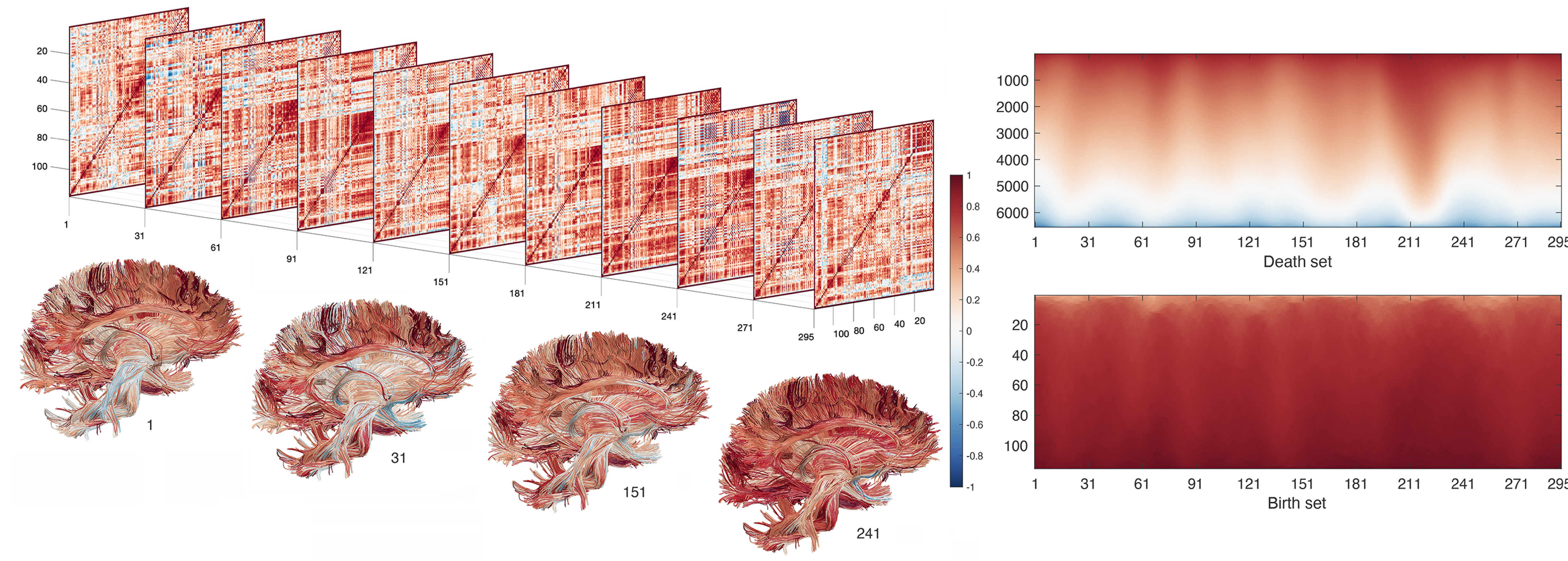

Fig. 2. Left: Dynamically changing correlation matrices computed using the sliding window of size 60 in rs-fMRI (Huang et al., 2020). The correlation matrices are superimposed on top of white matter fibers. Right: Topological embedding (birth-death decomposition) that is lossfree. Columns are the sorted birth and death edge values at that particular time point.

Wasserstein distance

The Wasserstein distance measuring 0D topology between graphs $\mathcal{X}_1$ and $\mathcal{X}_2$ is given by

$$\mathcal{D}_0(\mathcal{X}_1, \mathcal{X}_2) = \Big[\sum_{i=1}^{q_0} (b^1_{(i)} - b^2_{(i)})^2\Big]^{1/2},$$

where $b^j_{(i)}$ is the i-th smallest birth values in $\mathcal{X}_j$. The Wasserstein distance for measuring 1D topology is given by

$$\mathcal{D}_1(\mathcal{X}_1, \mathcal{X}_2) = \Big[\sum_{i=1}^{q_1} (d^1_{(i)} - d^2_{(i)})^2\Big]^{1/2},$$

where $d^j_{(i)}$ is the i-th smallest death values in $\mathcal{X}_j$. The combined topological distances

$$\mathcal{D}^2 = \mathcal{D}_0^2 + \mathcal{D}_1^2$$

is used for clustering.

Topological clustering

Given n graphs, we will cluster them into k clusters $C = (C_1, \cdots, C_k)$. We minimize the within-cluster topological distance

$$l_W(C) = \sum_{j=1}^{k} \sum_{X \in C_j} \mathcal{D}(X, \mu_j)$$

with the *topological mean* μ_j. The optimization is done in the two-step process of computing μ_j and minimizing cost l_W iteratively (Fig. 3).

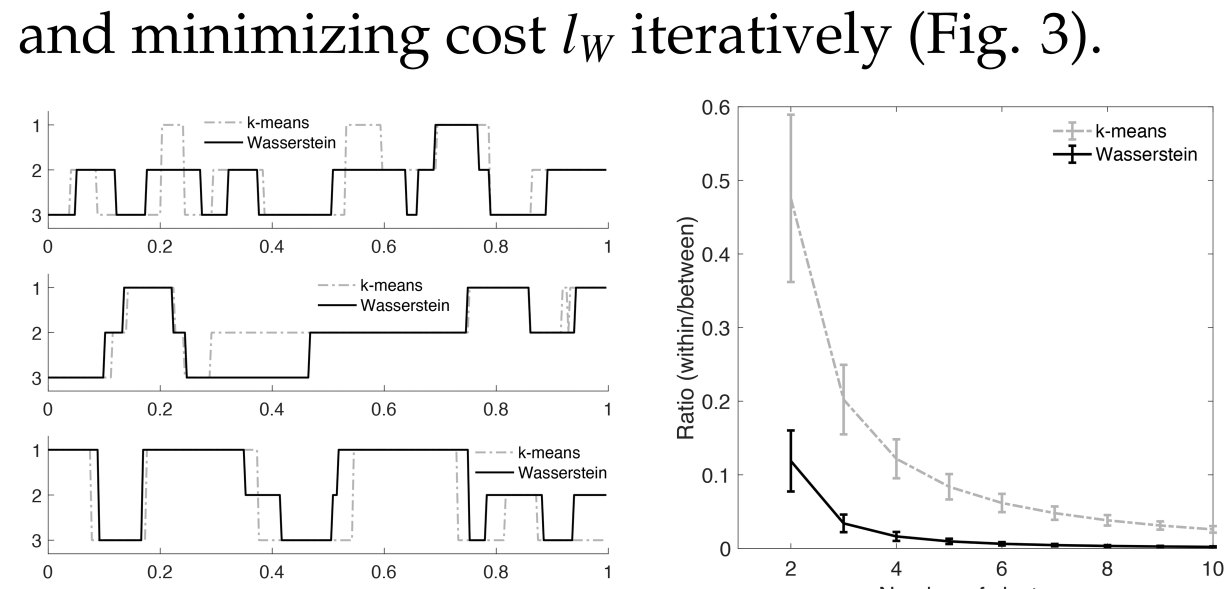

Fig. 3. The time series of estimated state space using the Wasserstein distance and k-means clustering for 3 subjects. The ratio of within-cluster to between-cluster distances. The ratio is 6 times smaller for the Wasserstein distance.

State space estimation

The 479 healthy subjects (ages 13 to 25 years) of the resting-state fMRI in the HCP database were used. The fMRI data were spatially averaged across voxels within 116 parcellations to obtain dynamically changing connectivity matrices (Chung et al., 2019), which is feed into topological clustering (Fig. 4).

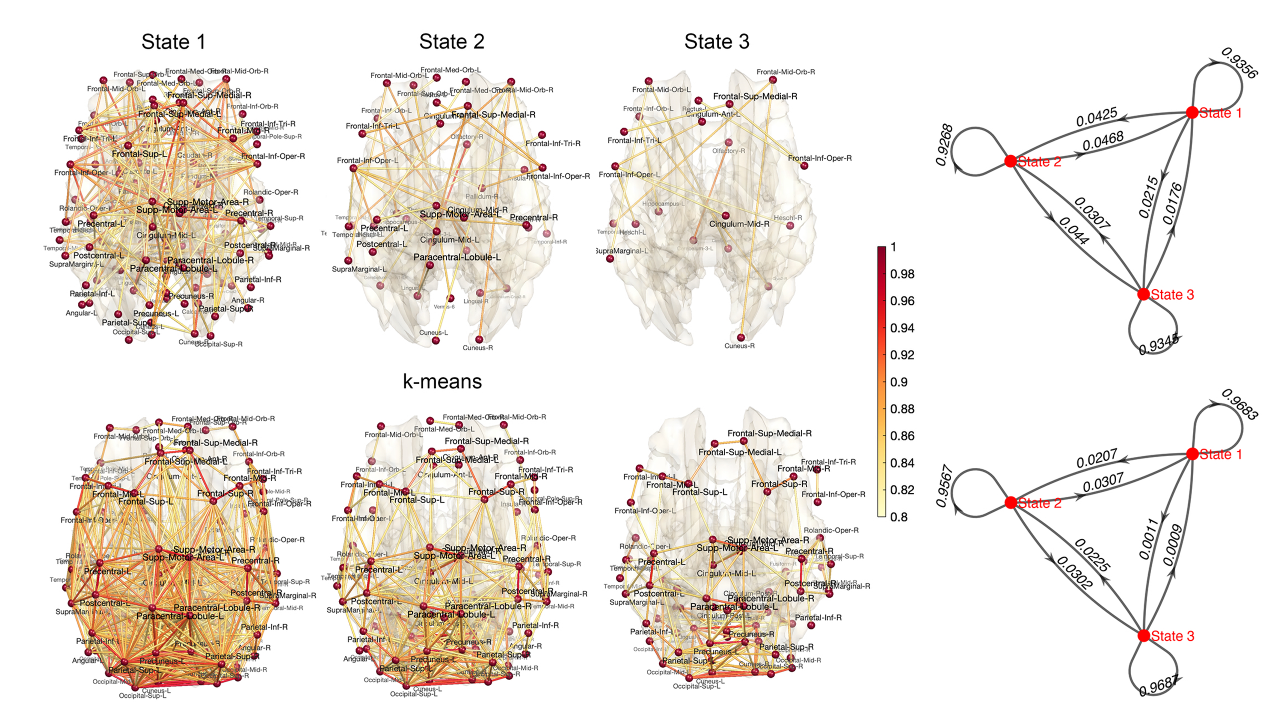

Fig. 4. The average estimated state spaces using the proposed topological clustering. The change of state space is modeled as a Markov chain. The Wasserstein distance significantly increases the transition probability to stay in the same state.

The dataset consists of 132 monozygotic (MZ) twin pairs and 93 same-sex dizygotic (DZ) twin pairs. We computed heritability index within each state (Fig. 5) (Chung et al., 2019).

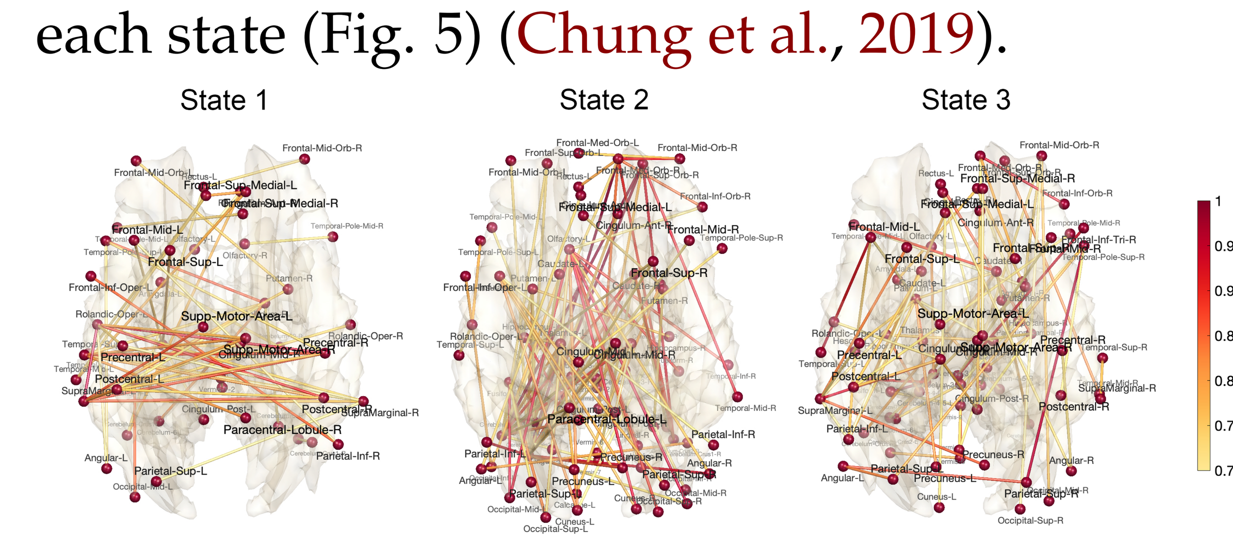

Fig. 5. The heritability index computed for each state showing extensive genetic contribution of dynamically changing state.

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