Graph Diffusion Distance: A Difference Measure for Weighted Graphs Based on the Graph Laplacian Exponential Kernel

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Introduction

We propose a novel difference metric, called the graph diffusion distance (GDD), for quantifying the difference between two weighted graphs with the same number of vertices.

- Our metric is based on measuring the average similarity of heat diffusion on each graph by means of the graph Laplacian exponential kernel.
- The GDD is defined as the Frobenius norm of the difference of the kernels, at the diffusion time yielding the maximum difference.

Motivation

The motivating principle behind our approach is the idea that two weighted graphs are similar if they enable similar patterns of information transmission.

Graph Diffusion Distance

- Let A_1 and A_2 be weighted adjacency matrices for N vertices, so both A_1 and A_2 are symmetric, non-negative, $N \times N$ real matrices with zeros along the principle diagonal. The Edge Difference Distance (EDD) is defined as $d_{edd}(A_1, A_2) = ||A_1 - A_2||_F$.
- The (unnormalized) graph Laplacian operator is defined according to [3]: $L_n = D_n - A_n$ (for $n = 1, 2$), where D_n is a diagonal degree matrix for the adjacency A_n, i.e. $(D_n)_{i,i} = \sum_{j=1}^{N} (A_n)_{i,j}$.
- Given two graphs represented by L_1 and L_2, the Laplacian exponential kernels are defined as $\exp(-tL_1)$ and $\exp(-tL_2)$.

The GDD

$$\xi_{gdd}(A_1, A_2; t) = ||\exp(-tL_1) - \exp(-tL_2)||_F^2$$
$$d_{gdd}(A_1, A_2) = \max_t \sqrt{\xi_{gdd}(A_1, A_2; t)}$$

where $||\cdot||_F$ is the matrix Frobenius norm.

Proposition

The GDD is a metric in the strict mathematical sense, i.e.
For any $N \times N$ adjacency matrices A, B, C
i) $d_{gdd}(A, B) \geq 0$, and $d_{gdd}(A, B) = 0$ iff $A = B$
ii) $d_{gdd}(A, B) = d_{gdd}(B, A)$
iii) $d_{gdd}(A, C) \leq d_{gdd}(A, B) + d_{gdd}(B, C)$

Edge Deletion Perturbation

The example below shows that the GDD is sensitive to the importance of the deleted edge. However, $d_{edd} = \sqrt{2}w$, regardless of the edge location (w is the edge weight).

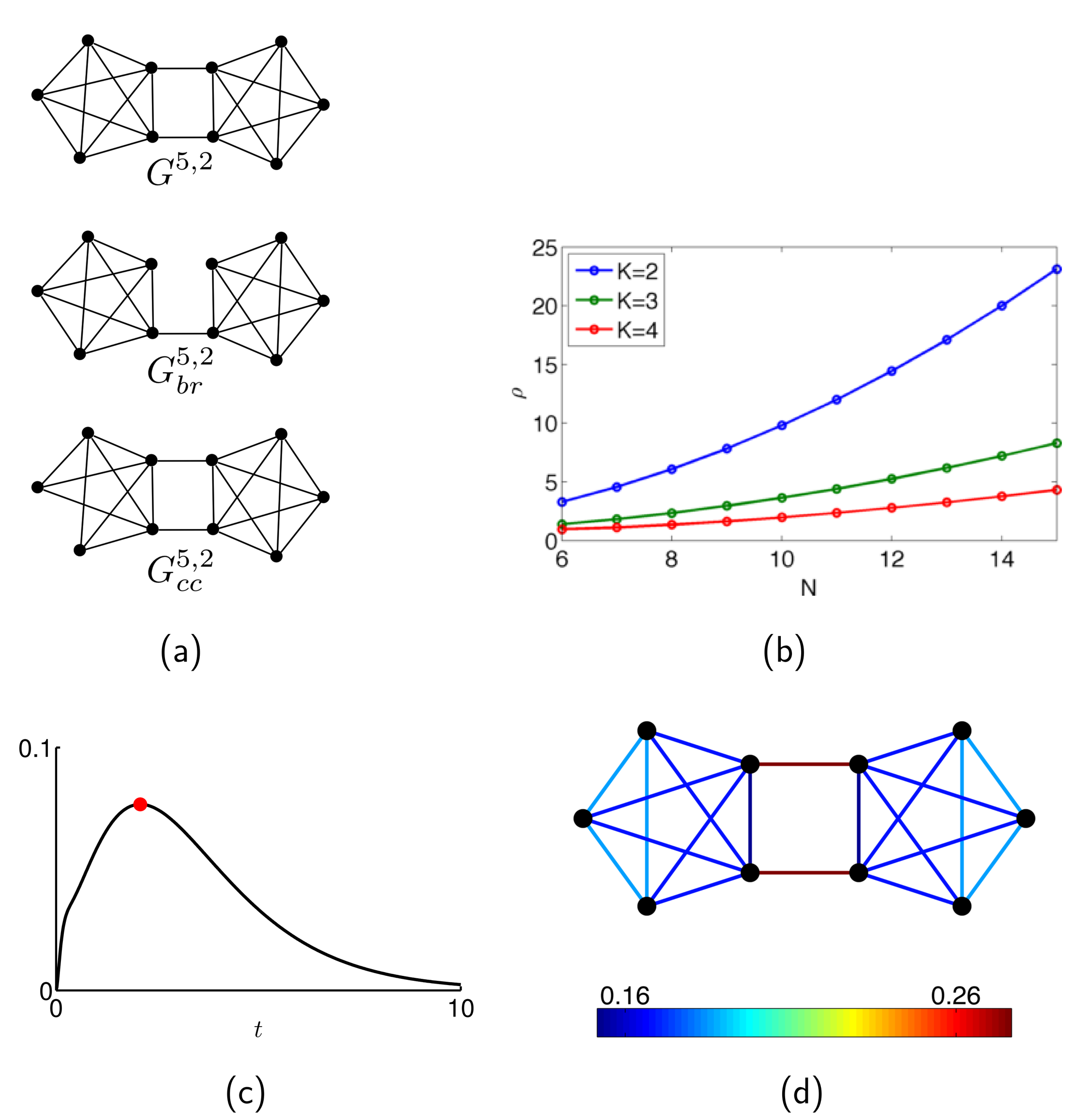

Figure 1: (a) Barbell graph, and single-edge perturbations, for $N = 5$, $K = 2$. (b) Plot of ratio $d_{gdd}(G^{N,2}, G^{N,2}_{br})/d_{gdd}(G^{N,2}, G^{N,2}_{cc})$ vs N. (c) Plot of $\xi(t)$ for $A_1 = G^{5,2}$, $A_2 = G^{5,2}_{cc}$, red dot indicates maximum, corresponding to $d_{gdd}(A_1, A_2)^2$. (d) Values of normalized edge deletion perturbation, on edges of $G^{5,2}$.

Brain Connectivity Graphs

Brain connectivity graphs are generated from diffusion MRI data using the following steps:

- In each voxel, a fiber orientation distribution (FOD) function is fit do the data using the method in [2].
- Axonal directions are extracted from the FOD by means of the tensor decomposition approach [1].
- A deterministic fiber tracking algorithm is used to integrate the axonal directions and generate brain connectivity map.
- We generate a brain connectivity graph using the procedure described in [4].

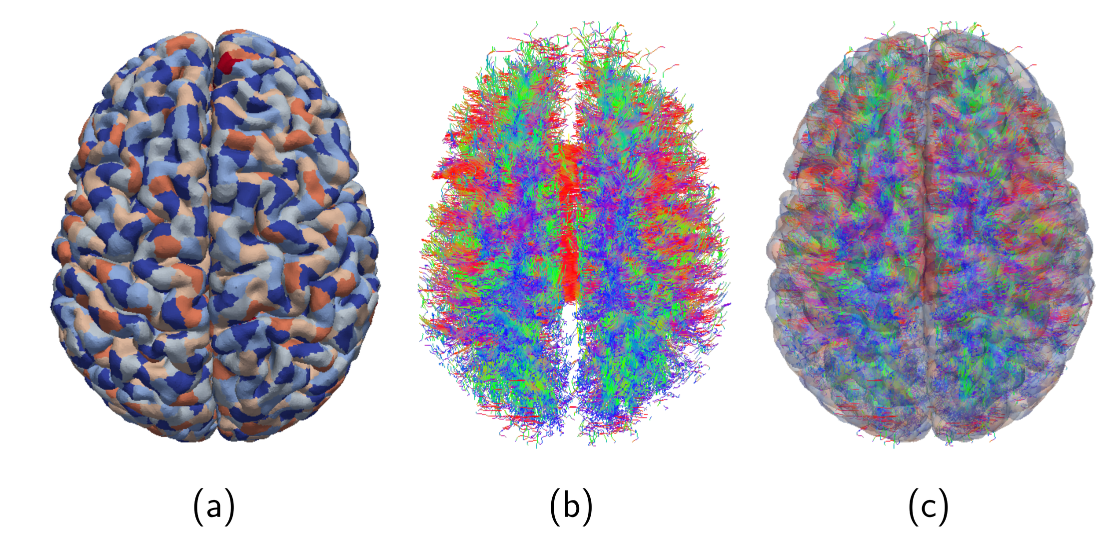

Figure 2: (a) Brain cortex. (b) Reconstructed axon bundles from diffusion MRI data. (c) Tracts and cortex superimposed.

Edge Deletion Perturbation - Brain Connectivity Graph

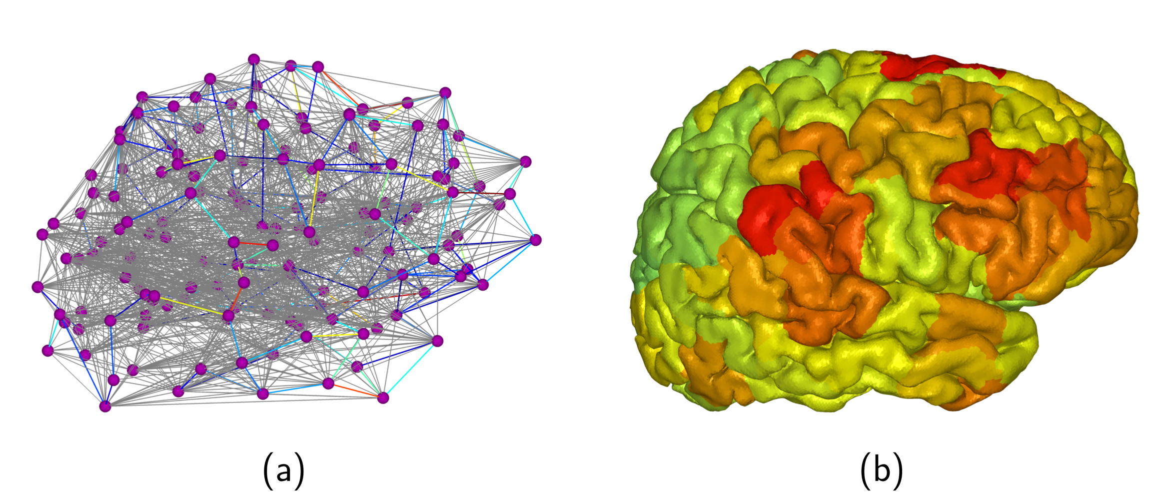

Figure 3: (a) Normalized edge-deletion perturbation, for brain connectivity graph (thresholded to show only top 10%). (b) Normalized EDP averaged over all edges incident to each vertex, rendered on cortical surface.

Undersampling Experiment

- We create subsets of the fully sampled by successively reducing the number of measurements.
- For each subset, we reconstruct a brain connectivity graph.
- The reconstructed graphs are used for comparison between EDD and GDD.

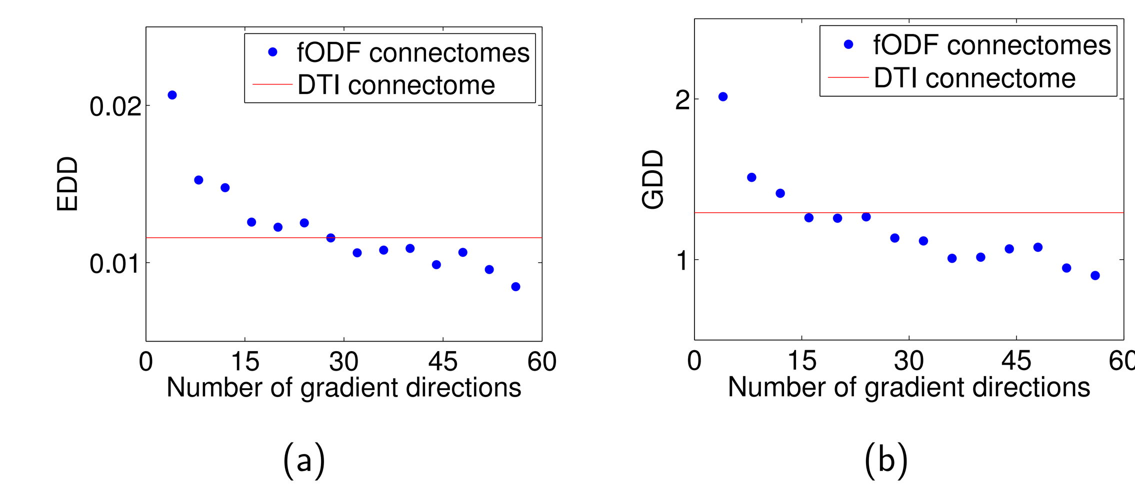

Figure 4: (a) GDD between A_{60} and A_n, where n is the number of diffusion weighted gradient directions used to compute the FODs. (b) Similar, but using EDD.

References

[1] F. Jiao, Y. Gur, and Chris R. Johnson, "Detection of crossing white matter fibers with high-order tensors and rank-k decompositions.", in IPMI'11, pp. 538-549, July 2011.

[2] Y. Weldeselassie, A Barmpoutis, and M. S. Atkins, "Symmetric positive-definite cartesian tensor orientation distribution functions (CT-ODF)", in MICCAI'10, pp. 582-589, 2010.

[3] F K Chung, "Spectral Graph Theory", vol. 92 of CBMS Regional Conference Series in Mathematics, AMS Bookstore, 1997.

[4] D K Hammond, B Scherrer, and S Warfield, "Cortical graph smoothing : a novel method for exploiting DWI-derived anatomical brain connectivity to improve EEG source estimation", IEEE Transactions on Medical Imaging, 32(10), pp. 1952-63, Oct. 2013.

Acknowledgements

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