Kernel Classification of Connectomes Based on Earth Mover’s Distance between Graph Spectra

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MRI acquisition  →  Network construction  →  Machine learning on networks

N examples of phenotype I

M examples of phenotype II

How to capture differences between the classes?
How to classify networks?

- **Graph embedding methods**
  - describe a network via a vector

- **Kernel classifiers**
  - define a positive semi-definite function on graphs and feed it to the SVM (support vector machines)
Kernel approach

N examples of phenotype I

M examples of phenotype II

A kernel on networks?

(N+M) x (N+M) Gram matrices (1 for each kernel)

Kernel SVM with 10 fold cross validation (100 runs with different splits)

Classification pipeline
A kernel on networks?

Provided we have a distance between the two networks $G_1$ and $G_2$, we can compute a kernel by:

$$K(G, G') = e^{-\alpha \omega(G, G')}$$

How to compute a distance between two connectomes?
Idea

Use spectral distributions of the normalized graph Laplacians to capture differences in the structure of connectomes.
What is a normalized Laplacian?

Let $A$ be a graph adjacency matrix

$D$ is a diagonal matrix of weighted node degrees:

$$d_i = \sum_j a_{i,j}$$

Graph Laplacian is:

$$L = D - A$$

Normalized graph Laplacian is:

$$\mathcal{L} = D^{-1/2}LD^{-1/2}$$
Why its spectra are so special?

The eigenvalues are in range from 0 to 2:
- can compare networks with different sizes
- no need to normalize networks

The shape of the eigenvalue distribution, its symmetry and the multiplicity of particular values capture information about graph structure

Chung F. (1997) Spectral Graph Theory
Graph structure in spectral distributions

Distance between spectral distributions?

Could use measures from information theory
- need density reconstruction

An idea behind the earth mover's distance (EMD):

If each distribution is represented by some amount of dirt, EMD is the minimum cost required to move the dirt of one distribution to produce the other. The cost is the amount of dirt moved times the distance by which it is moved.

**Pipeline**

- **N** examples of phenotype I
- **M** examples of phenotype II
- Take the normalized Laplacians
- Compute the spectra
- Measure the EMD between spectral distributions
- \((N+M) \times (N+M)\) Gram matrices (1 for each kernel)
- Kernel SVM with 10 fold cross validation (100 runs with different splits)

**Classification pipeline**
Example dataset: UCLA Autism

- structural connectomes
- 94 subjects
- 51 ASD subjects (age 13 ± 2.8 years),
  43 TD subjects (age 13.1 ± 2.4 years)
- 264x264 matrices
deterministic tractography (FACT)


UCLA Autism: spectral distributions

Spectra of the group average matrices

Spectra of the individual matrices of TD class
UCLA Autism: classification

- Run parallel analysis on connectomes with three different weighting schemes:
  - weights proportional to the number of streamlines
  - weights proportional to the inverse Euclidean distance between the centers of the respective regions
  - combined the above weights

- Compare performance of the proposed pipeline against the linear SVM classifiers on the vectors of edges and the vectors of sorted eigenvalues.

- Area under the ROC-curve (ROC AUC), 10-fold cross-validation, 100 runs with different splits
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**UCLA Autism: results**

![Box plot showing ROC AUC for different kernel methods and edge weights.](image-url)
**UCLA Autism: results**

Gram matrix based on the EMD between the normalized Laplacian spectra: the TD group shows larger variability

Precision and recall values: Algorithm performs quite well identifying ASD subjects, but tends to classify TD subjects as pathological
Conclusions

- Spectral distributions of the normalized Laplacians capture some meaningful **structural properties** of brain networks which make them different from other network classes.

- Spectral distributions of connectomes can help to **distinguish normal and pathological brain networks**.

- **Further studies are needed** to explore whether these findings generalize to other classification tasks and other schemes of network construction.
Thank you!

Q?

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