Homological information to refine small-world regime of brain functional connectivity networks

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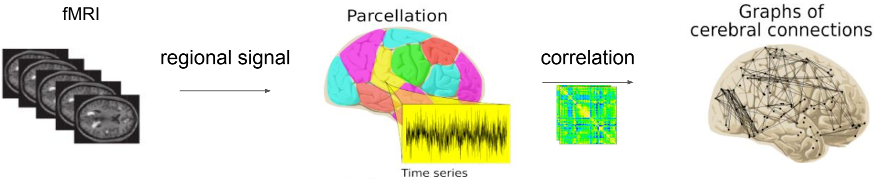
Motivations

- Topological Data Analysis is a powerful tool for extracting information in Networks
- Homology uses information between local and global scale
- Comparison with synthetic constructions can help understand properties of real datasets
- Application to functional brain connectivity networks



Goals

Our goals are to:

- Find a measure of mesoscale efficiency of brains and compare it to Watts-Strogatz graphs
- Predict the proportion of long range links using Topological Data Analysis, in terms of predicting the p of Watts-Strogatz graphs

Presentation of the datasets

We used two different datasets:

1. 37 matrices of dimension 90×90 (AAL90), 17 comatose patients, 20 healthy volunteers;
2. 200 matrices of dimension 90×90 (AAL90) all from healthy volunteers.

Given a threshold or a sparsity value, we extract a graph representation of the data, considering as connected the most correlated nodes.

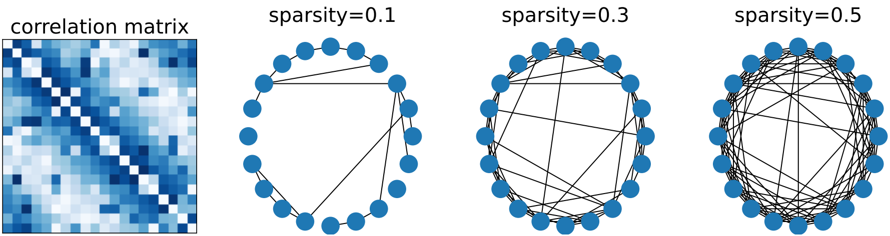


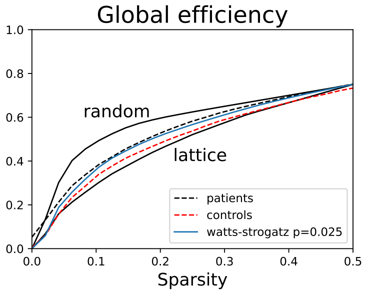
Figure: Example of graph extraction from a synthetic matrix 20×20

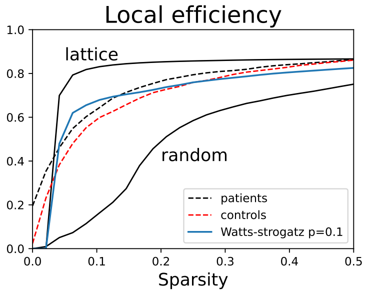
Small World properties of Brain Functional Networks

In (Achard, Bullmore, 2007) network efficiency measures on brain functional networks are studied. Efficiency is defined as

$$E_{glob} := \frac{1}{N(N-1)} \sum_{i \neq j \in G} \frac{1}{L_{i,j}} \qquad E_{loc} := \frac{1}{N_{G_i}(N_{G_i}-1)} \sum_{j \neq k \in G_i} \frac{1}{L_{j,k}}$$

Brain data have *global efficiency* similar to a Watts-Strogatz with $p = 0.025$ and *local efficiency* similar to a Watts-Strogatz with $p = 0.1$.





Watts–Strogatz model

Watts-Strogatz construction is our benchmark for synthetic small world graphs.

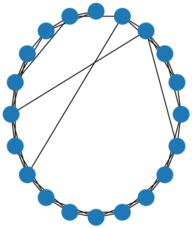
Watts–Strogatz model

- start with a ring lattice;
- Rewire every edge with fixed probability p.

Observation

- If $p = 0$ ring lattice
- if $p = 1$ random

Figure: Watts-Strogatz graph with 20 nodes and $p = 0.05$



Simplicial Complex

Simplicial Complex

A k-simplex is the convex hull of its $k+1$ vertices.

A simplicial complex $\mathcal{K}$ is a set of simplices s.t.

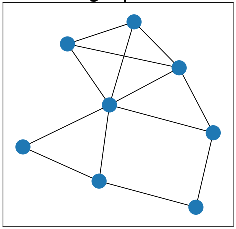
1. Every face of a simplex from $\mathcal{K}$ is also in $\mathcal{K}$.
2. Intersection of any two simplices $\sigma_1, \sigma_2 \in \mathcal{K}$ is a face of both σ_1 and σ_2.

k-chains

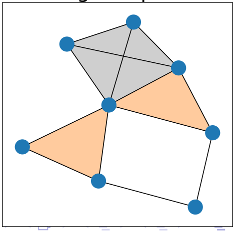
Multidimensional extension of paths.

S simplicial complex. A simplicial k-chain is a finite formal sum $\sum_{i=1}^{N} c_i \sigma_i$ where $c_i \in \mathbb{Z}$, σ_i of oriented k-simplex.

graph



flag complex



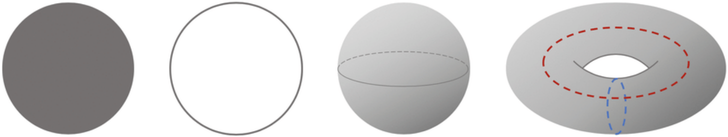
Homology groups and Betti numbers

Homology groups and betti numbers

Homology groups defined as:

- $H_k := \ker\partial_k / \mathrm{im}\partial_{k+1}$
- Betti numbers $\beta_k := \mathrm{rank} H_k$

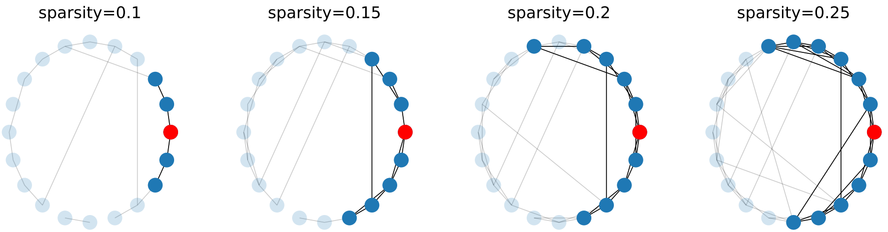
Intuition: k-th homology group as the group generated from k-dimensional voids. The number of voids are the Betti numbers



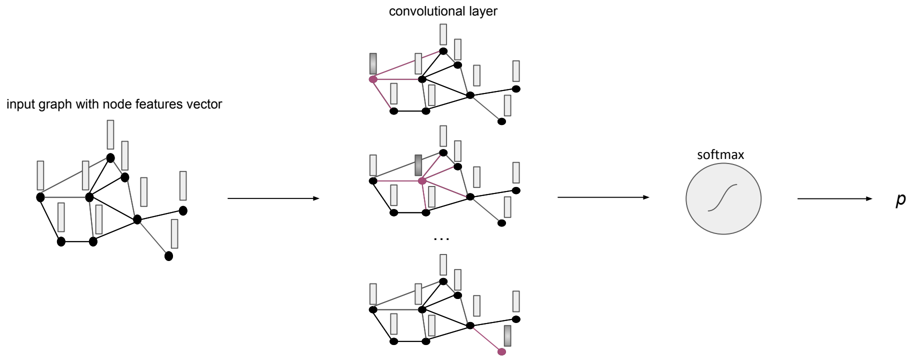
$\beta_0 = 1$	$\beta_0 = 1$	$\beta_0 = 1$	$\beta_0 = 1$
$\beta_1 = 0$	$\beta_1 = 1$	$\beta_1 = 0$	$\beta_1 = 2$
$\beta_2 = 0$	$\beta_2 = 0$	$\beta_2 = 1$	$\beta_2 = 1$

Feature Vector

- For each node, we computed the "2-steps" neighborhood for 10 different sparsity levels
- For each of the 10 neighborhoods, we computed the 1-dimensional Betti number
- For each node, we define as feature vector the vector of these 10 Betti numbers



GCN Model and training

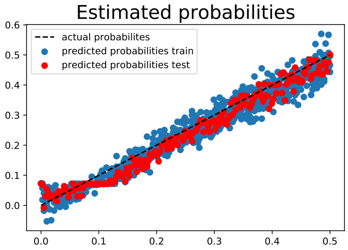


Tool to do regression for graph structured data: Graph Neural Network

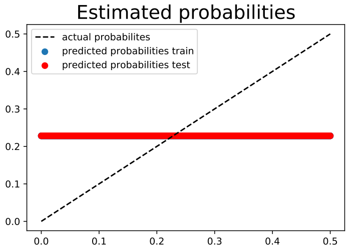
- GCN model is trained over a dataset of $n = 1000$ Watts-Strogatz with chosen with p taking values in $[0, 0.5]$
- The trained model is then applied to the brains dataset

Results on Watts-Strogatz networks

RMSE on the test set is lower than 0.02.
A second, identical model is trained for reference, using vectors of ones instead of topological features. We will refer to this model as *null model*.



(a) homology informed model

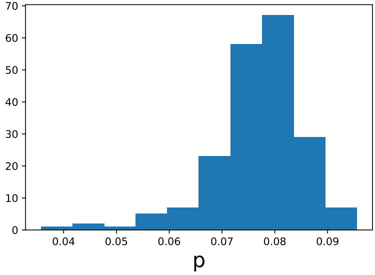


(b) null model

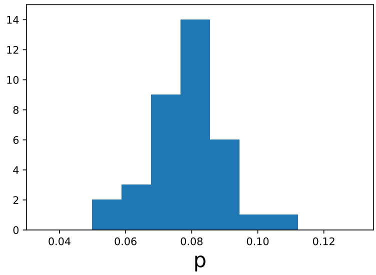
Figure: Results on Watts-Strogatz Graphs

Results on Brain Networks

- Model applied to real data always predicts a probability (!)
- Prediction on brains has mean around 0.077: between the local 0.1 and global prediction 0.025



(a) HCP Dataset



(b) Coma Dataset

Figure: Histogram of estimated probabilities on brain functional connectivity networks

Conclusions and future outlooks

Our work suggests the following:

- Homological information can be cast as useful features in a task over brain functional connectivity networks
- A measure of mesoscale efficiency can be obtained by using the predicted rewiring probability extracted by the GNN.

There may be several future directions in our work,

- Training on the synthetic dataset to do transfer learning on a classification task
- Results on finer representations of brain connectivity

Thank you!

Thank you for your attention!

Contacts and code

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https://github.com/SimoneChiominto/TDA_BrainNetworks.git