Neighborhoods for classifying binary dynamics in directed networks with machine learning

LU Interdisciplinary Applied Mathematics seminar

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Overview

About.

- ▶ Based on work in preparation (2019-2021)
- In collaboration with the Blue Brain Project (EPFL)
- ► Funded by EPSRC grant "Topological Analysis of Neural Systems"

Goals.

- ▶ Neurological: Make a *in silico* model of a brain based on *in vivo* models.
- ▶ Mathematical: Distinguish neurological activity by its topological features.

Plan.

- Neuroscience
 - Structure of the network
 - Experiments on the network
- 2. Mathematics
 - ► Topology in neuroscience
 - Neighborhoods in a digraph
- 3. Implementation and results
 - Classification by machine learning
 - Computational requirements

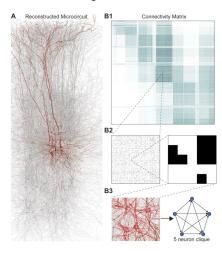
Neuroscience: Structure

Microcircuit of a rat somatosensory column, average over 6 instances:

	neuroscience	mathematics
31 346	neurons	vertices
7 803 528	synapses	directed edges

This graph is:

- ► Biologically modeled ("grown")
- ► Very sparse (0.8% density)
- ► Physically small (0.29mm³ of brain)
- Relatively small (newest version has 4.2 million neurons and 4.8 billion synapses)
- Open source (available at bbp.epfl.ch/nmc-portal)
- Not a random graph (more topological features)



Neuroscience: Structure

The complexity of a network can be considered via the number of *cliques*.



undirected 3-clique



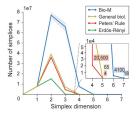
directed unordered 4-clique

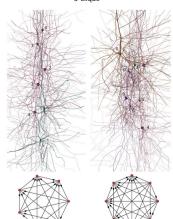


directed ordered 5-clique

Large cliques unlikely, and among those unordered cliques dominate. On *n* vertices:

- ▶ $3^{n(n-1)/2}$ possible configurations
- ▶ 2^{n(n-1)/2} possible configurations as directed *n*-cliques
- n! possible configurations as directed ordered n-cliques





Neuroscience: Experiments

Activity.

- Each neuron has an *electric potential* and a *threhsold*.
- If the potential passes the threshold, the neuron fires and sends its potential along outgoing synapses.
- Each synapse has a probability of signal *transmission*.
- Modern models encode plasticity, or the change in future transmission probability based on past transmission.

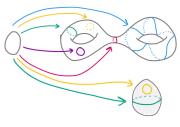


Experiments.

- External input is connected by *thalamic fibers* to receptory neurons.
- ▶ Different *stimuli* are sent to the brain (flick of a whisker)
- ▶ The propogation of activity is recorded over 250ms after the input of the signal
- ▶ 8 stimuli, 557 repetitions of each
- ▶ Data recorded as a list of values (n_i, t_i) of the neuron index and the time it fires

Mathematics: Topology

- ▶ The *topology* of a space X is reflected by classes of maps $S^n \to X$.
- ▶ The more (homotopy) classes in C_n , the more complex the space.
- The flag complex of a directed graph comes from associating to every directed n-clique an (n − 1)-dimensional simplex.





homology groups:
$$H_n(X) = \ker(C_n \to C_{n-1})/\operatorname{im}(C_{n+1} \to C_n)$$

Betti numbers: $\beta_n(X) = |H_n(X)|$

Euler characteristic: $\chi(X) = \beta_0 - \beta_1 + \beta_2 - \beta_3 + \cdots$

normalized Betti coefficient:
$$\mathfrak{B}(X) = \frac{\beta_0(X)}{\# \text{ of vertices}} + \frac{2\beta_1(X)}{\# \text{ of edges}} + \cdots$$

Mathematics: Neighborhoods in a digraph

Neuroscience uses the *firing rate* of a neuron or region for classification. We use different parameters based on graph neighborhoods.

- ▶ Fundamental: firing rate, in degree, out degree, recioprocal connection count
- ► Algebraic: clustering coefficient
- ▶ Topological: Euler characteristic, Betti coefficient, density coefficient
- ► Spectral: adjacency, Laplacian, transition probability



In total 30 different parameters.

Implementation: Technical requirements

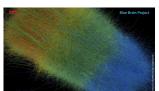
Neuroscience: EPFL

- Circuit built and experiments run on EPFL Blue Brain Project supercomputers
- 42k cores, 94TB of RAM
- ► Takes about 10 hours to simulate 250ms

Mathematics: University of Aberdeen

- Analysis run on UoA Maxwell HPC
- ▶ 1.2k cores, 12TB of RAM
- Takes about 2 hours to featurize each parameter, 1 minute to classify
 - Requests 40 cores, 150GB of RAM
 - Topological computations in parallel







References.

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