Setting the Stage with Networks and Network Dynamics

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Abstract

- To help set the mathematical stage for the workshop, I will briefly present some fundamental ideas in networks and network dynamics. I will discuss various types of networks (such as directed networks, multilayer networks, and so on), with an aim towards trying to convey what we do and don't know how to do. In this vein, I will also comment about dynamics on networks, dynamics of networks, and networks that coevolve with dynamics.
- I plan to use roughly half of the allotted time for my presentation slides, and I expect active discussions and audience questions for the other half.
- Springboarding from these discussions, we should try to set the stage for formulating interesting and concrete projects at the conclusion of the workshop.

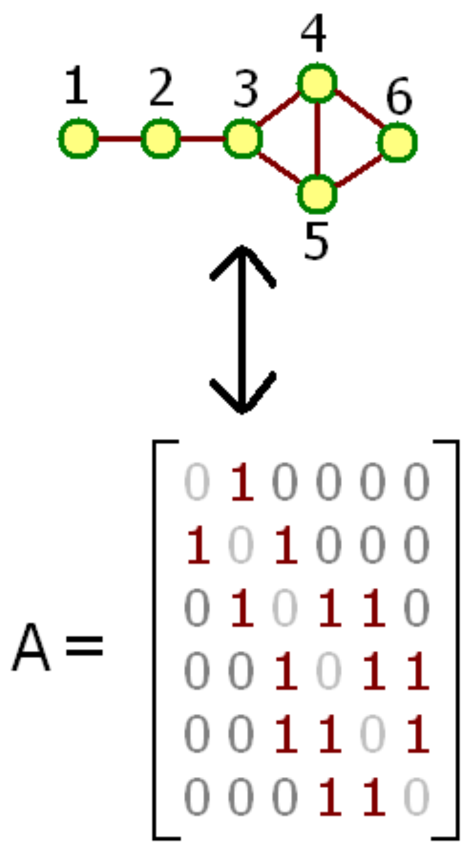
Interrupt me with questions!

This is supposed to be a discussion to help set the stage for the workshop.

Two Flavors of Issues when Generalizing Network Representations and Data Structures

- 1. There are many different ways to generalize some approach or quantity (betweenness centrality, clustering coefficient, etc.) and many different choices to make in the process, so we need to think about which way to do it and what is most appropriate for a given problem.
  - Example: Given a weighted network (with larger weights encoding stronger relationships), how do we want to measure the distances of a walk on the network?
- 2. When generalizing, we lose some convenient feature (e.g., a important theorem no longer applies) and then we need to figure out — through development of theory and/or methods — how to get the generalization to work.
  - Example: The adjacency matrix of a directed network is generically asymmetric, so the leading eigenvalue is no longer guaranteed to be real, and spectral methods that rely on having a real leading eigenvalue or leading eigenvector need to be adjusted.

Graphs: The Simplest Networks

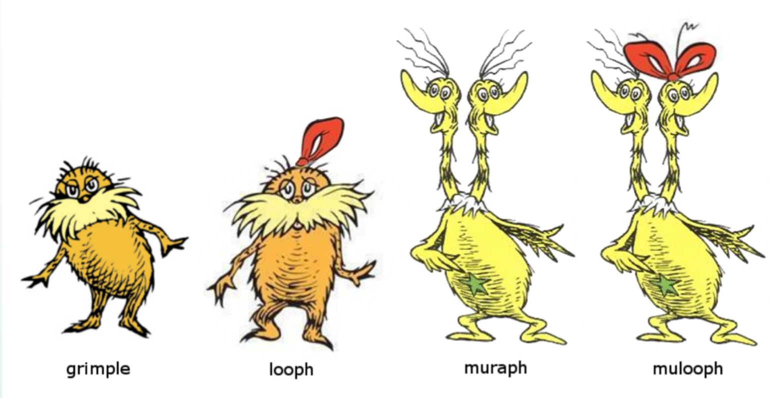


- Remark: In much networks literature, it is common to use the word "networks" in a way that does not automatically include dynamics. This is different in some other traditions.
- Adjacency matrix ***A***
  - $A_{ij} = 1$ if there is a connection between nodes i and j
  - $A_{ij} = 0$ if no connection
- We can generalize these representations to account for edge directions, edge weights, multiple relationships, changes with time, and other complications.
- Some things that we like:
  - Generative models of random graphs, local clustering coefficient, centrality measures (to measure importance of nodes and edges), community structure and other mesoscale properties, etc.
  - How do we generalize them for more complicated network representations?

Configuration-Model Random Graphs

- Bailey K. Fosdick, Daniel B. Larremore, Joel Nishimura, & Johan Ugander [2018], "Configuring Random Graph Models with Fixed Degree Sequences", SIAM Review, Vol. 60, No. 2: 315–355

- Fix degree sequence and connect stubs (i.e., ends of edges) to each other uniformly at random
  - Or fix a degree distribution and draw a degree sequence from it
- Self-edges and multi-edges?
- Null model in community detection



Graph Laplacian Matrices

- Naoki Masuda, MAP, & Renaud Lambiotte [2017], "Random Walks and Diffusion on Networks", *Physics Reports*, Vol. 716–717: 1–58
  - Combinatorial graph Laplacian: $L = D - A$
  - Random-walk normalized Laplacian: $D^{-1}L$
- Spectral clustering: Use eigenvalues and eigenvectors of a Laplacian or related matrix (e.g., a modularity matrix)

Weighted Networks

- Note: Technically, these are edge-weighted networks, which is what people usually mean when they say "weighted networks". One can also think about node weights.
- Weights versus "distances"
  - In a *weight matrix* (i.e., weighted adjacency matrix), larger values indicate stronger connections
  - In a *distance matrix*, larger values indicate weaker connections
  - Data may arise most naturally as costs (i.e., "distances") or as weights
- If you are given weights, how do you measure distances, such as for walks on networks and anything (e.g., centrality measures like betweenness) that use them?
- Weighted generalizations of ideas like local clustering coefficients: How should you normalize?
- Conceptual trickiness in generalizations of random-graph models: shuffling edges versus redistributing weights?
  - For example, in generalizations of configuration models and stochastic block models
  - Conceptually harder than some other generalizations (e.g., multilayer networks) that are often harder for other things

Directed Networks

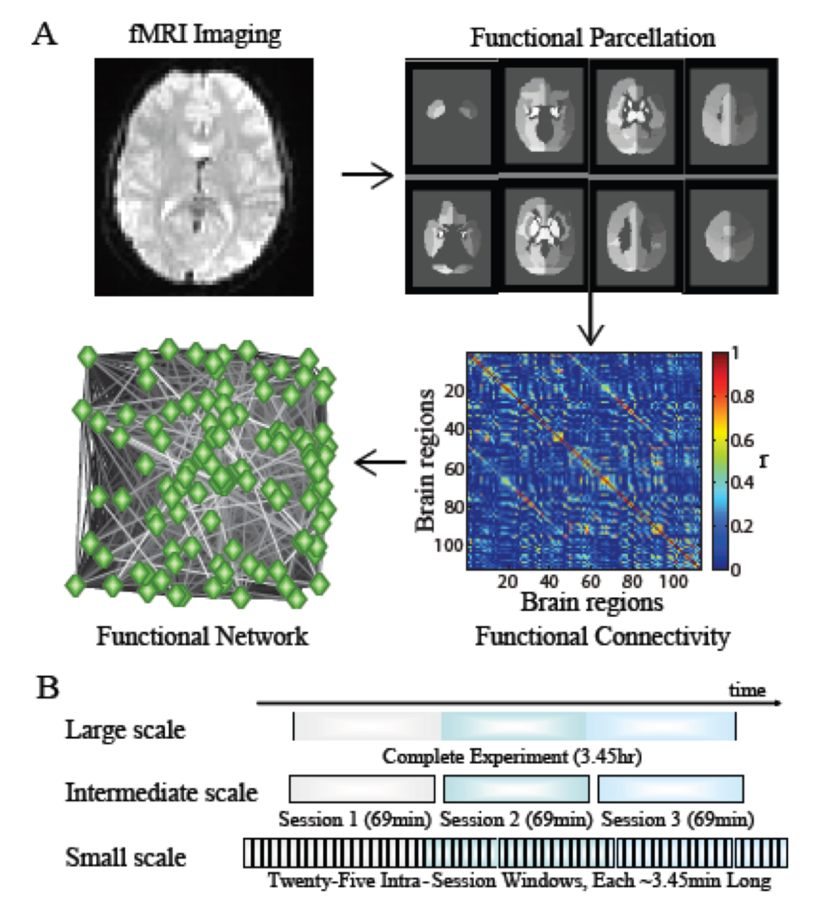
- Fragkiskos D. Malliaros & Michalis Vazirgianis [2013], "Clustering and Community Detection in Directed Networks: A Survey", *Physics Reports*, Vol. 533, No. 4: 95–142
- Graph Laplacians: out-degree versus in-degree

$$L' \equiv D^{-1}L = I - T\,.$$

That is, $(L')_{ij} = \delta_{ij} - (A_{ij}/s_i^{\text{out}})$.

- The leading eigenvalue and leading eigenvector are no longer typically guaranteed to be real, so spectral approaches need to be generalized to account for that
- Generalizing ideas like local clustering coefficients and network "motifs" to directed networks?
- Null models for community detection through directed generalization of configuration-model networks
  - Or use statistical-inference methods, such as with degree-corrected stochastic block models
  - Or use local methods, such as via personalized PageRank (although many of these methods want a real leading eigenvalue)

Signed Networks



- Naoki Masuda, Zachary M. Boyd, Diego Garlaschelli, & Peter J. Mucha [2023], “Correlation Networks: Interdisciplinary Approaches Beyond Thresholding”, arXiv:2311.09536
- Positive and negative edges
- Examples: Correlations, excitatory versus inhibitory dynamics, etc.
- Community structure and random-graph null models
  - A signed generalization of configuration models
- Spectral properties of adjacency and Laplacian matrices?
  - Difficulties in generalizing centrality measures (including not usually having a guarantee of a real, positive leading eigenvalue)
- Schematic from Danielle S. Bassett, Nicholas F. Wymbs, MAP, Peter J. Mucha, Jean M. Carlson, & Scott T. Grafton [2011], “Dynamic Reconfiguration of Human Brain Networks During Learning”, *Proceedings of the National Academy of Sciences of the United States of America*, Vol. 108, No. 18: 7641–7646
  - For imaging data: Threshold weights to obtain an unweighted network, making all weights positive somehow, or using signed weighted networks?
  - This paper does not consider signed-network methods

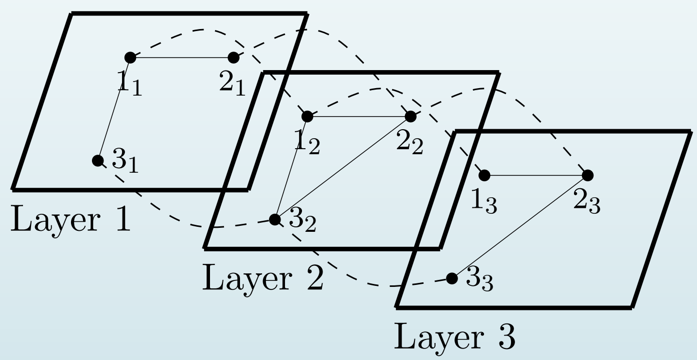
Networks with Complex-Valued Weights

- Lucas Böttcher & MAP [2024], "Complex Networks with Complex Weights", *Physical Review E*, in press (arXiv: 2212.06257)
- Applications include quantum walks on networks, graph signal processing, graph neural networks, transmission-line networks, coupled-oscillator networks, etc.
- Hermitian versus non-Hermitian matrices
- Need much more network analysis to generalize our favorite ideas to this setting
- Further studies using ideas like pseudospectra and non-normal matrices should be useful (e.g., for generalizing ideas like eigenvector centrality)
  - Lucas wanted me to ask if any folks at the workshop have some ideas to share

Multilayer Networks

(note: different use of the term than in machine learning)

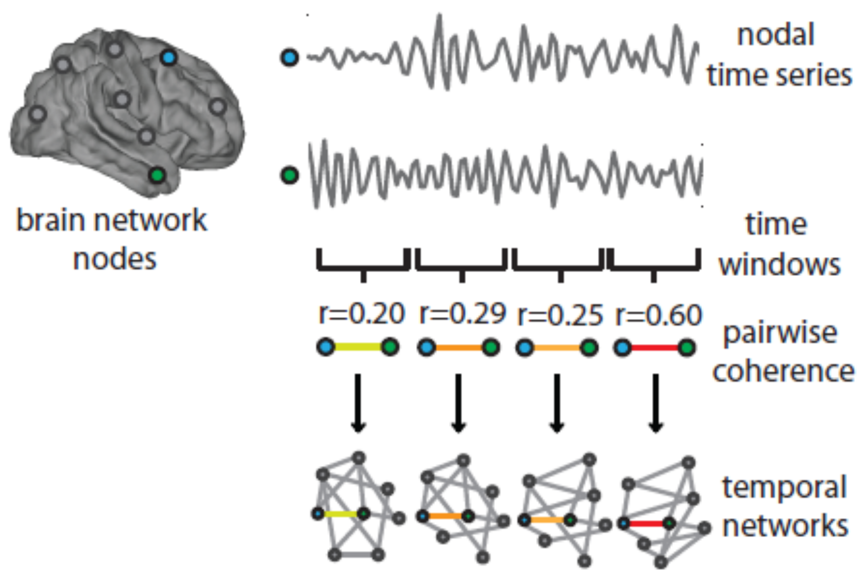
- Mikko Kivelä, Alex Arenas, Marc Barthelemy, James P. Gleeson, Yamir Moreno, & MAP [2014], "Multilayer Networks", *Journal of Complex Networks*, Vol. 2, No. 3: 203–271
- Manlio De Domenico [2022], *Multilayer Networks: Analysis and Visualization*, Springer International Publishing, Cham, Switzerland
- Adjacency tensor versus "flattening" into a supra-adjacency matrix
- Intralayer edges versus interlayer edges: Often less reliable data and more conceptual difficulties with the latter (what do the **ω** mean?)

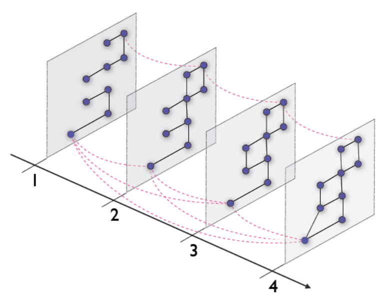


$$\longleftrightarrow \left[\begin{array}{ccc|ccc|ccc} 0 & 1 & 1 & \omega & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & \omega & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & \omega & 0 & 0 & 0 \\ \hline \omega & 0 & 0 & 0 & 1 & 1 & \omega & 0 & 0 \\ 0 & \omega & 0 & 1 & 0 & 1 & 0 & \omega & 0 \\ 0 & 0 & \omega & 1 & 1 & 0 & 0 & 0 & \omega \\ \hline 0 & 0 & 0 & \omega & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & \omega & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & \omega & 0 & 1 & 0 \end{array}\right]$$

- Schematic of "flattened" representation (as a supra-adjacency matrix) from M. Bazzi, MAP, S. Williams, M. McDonald, D. J. Fenn, & S. D. Howison [2016] *Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal*, **14**(1): 1–41

Multilayer Networks





- Top schematic from D. S. Bassett, N. F. Wymbs, M. Puck Rombach, MAP, P. J. Mucha, & S. T. Grafton [2013], *PLoS Computational Biology*, Vol. 9, No. 9: e1003171
- Bottom schematic from P. J. Mucha, Thomas Richardson, Kevin Macon, MAP, & Jukka-Pekka Onnela [2010], *Science*, Vol. 328, No. 5980: 876–878

- Tradeoffs here and also for the other more complicated representations:
  - Generalizing methods versus losing information?
  - Trustworthy data that jibes with these more complicated representations?
    - E.g., interlayer edge weights
- Multilayer representation of time-dependent networks
- Much state-of-the-art research is in trying to generalize familiar network concepts
  - Random-graph models, Laplacians, walks, centralities, clustering coefficients, etc.
    - E.g., eigenvector-based centralities (such as multilayer PageRank) where you can construct things in a way to still use Perron–Frobenius theorem and guarantee a real and positive leading eigenvalue
  - How do more complicated network structures affect dynamics on networks?

Polyadic (i.e., Higher-Order) Relationships

- Christian Bick, Elizabeth Gross, Heather A. Harrington, & Michael T. Schaub [2023], "What Are Higher-Order Networks", *SIAM Review*, Vol. 65, No. 3: 686–731
- Federico Battiston, Giulia Cencetti, Iacopo Iacopini, Vito Latora, Maxime Lucas, Alice Patania, Jean-Gabriel Young, & **Giovanni Petri** [2020], "Networks Beyond Pairwise Interactions: Structure and Dynamics", *Physics Reports*, Vol. 874: 1–92
- Hypergraphs and simplicial complexes
  - Generalizing structural measurements and analysis
    - E.g., generalizations of Laplacians (e.g., Hodge Laplacian)
  - How do polyadic interactions affect dynamics?
    - Modeling choice: Simplicial complexes (which require downward closure) versus hypergraphs?
- Topological data analysis (TDA)
  - See Moo Chung's talk this afternoon for tutorial on TDA

Networks and Dynamics

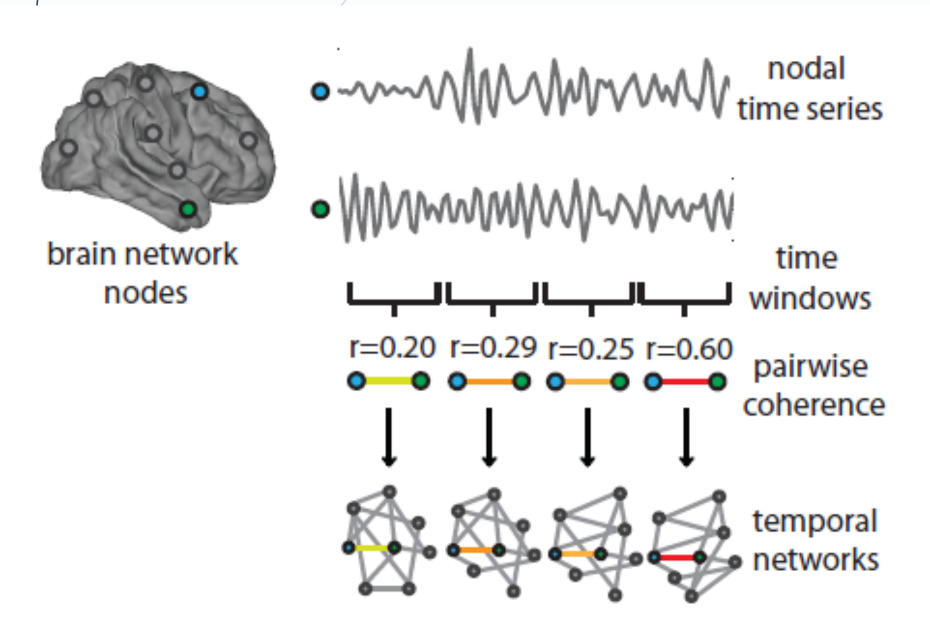
Dynamics on Networks

- MAP & J. P Gleeson [2016], "Dynamical Systems on Networks: A Tutorial", *Frontiers in Applied Dynamical Systems: Reviews and Tutorials*, Vol. 4, Springer International Publishing, Cham, Switzerland
- Much more specific topic: Stephen Coombes, Mustafa Sayli, Rüdiger Thul, Rachel Nicks, MAP, & Yi Ming Lai [2023], "Oscillatory Networks: Insights from Piecewise-Linear Modelling", *SIAM Review*, in press (arXiv2308.09655)
  - Includes models of neuronal dynamics on networks
- How does network structure affect dynamics on a network?
  - Faster synchronization for some types of networks? Slower flow of something on some networks?
- Coupled phase oscillators (e.g., Kuramoto model):

$$\dot{\theta}_i := \frac{d\theta_i}{dt} = \omega_i + \sum_{j=1}^{N} b_{ij} A_{ij} f_{ij}(\theta_j - \theta_i)\,, \qquad i \in \{1, \ldots, N\}\,,$$

- Better-developed theory for autonomous systems than for nonautonomous systems
  - E.g., One needs to generalize ideas like stable and unstable manifolds for nonautonomous systems
- Deterministic or stochastic dynamical processes
- Dynamics on combinatorial networks versus dynamics on 'metric networks'

Dynamics of Networks



- Petter Holme & Jari Saramäki [2012], "Temporal Networks", *Physics Reports*, Vol. 519, No. 3: 97–125
- Petter Holme [2015], "Modern Temporal Network Theory: A Colloquium", *European Physical Journal B*, Vol. 88, No. 9: 234
- Discrete time versus continuous time
  - Chopping up time series?!? (oy vey)
- Multilayer representation of temporal networks, with e.g. generalizing eigenvector-based centralities and community-detection methods

Adaptive (i.e., Coevolving) Networks

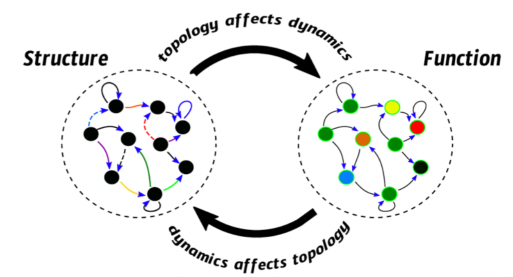


Fig. 1. Adaptive dynamical networks.

- Rico Berner, Thilo Gross, Christian Kuehn, Jürgen Kurths, & Serhiy Yanchuk [2023], "Adaptive Dynamical Networks", *Physics Reports*, Vol. 1031: 1–59
- Coupling between dynamics on networks and dynamics of networks
- Adaptive network weights:

$$\dot{\boldsymbol{x}}_i = f_i(\boldsymbol{x}_i, t) + \sum_{j=1}^{N} \kappa_{ij} g(\boldsymbol{x}_i, \boldsymbol{x}_j, t),$$

$$\dot{\kappa}_{ij} = h(\boldsymbol{x}_i, \boldsymbol{x}_j, t),$$

- Adaptive time delays (less well-studied?):

$$\dot{\boldsymbol{x}}_i(t) = f_i(\boldsymbol{x}_i(t), t) + \sum_{j=1}^{N} \kappa_{ij} g(\boldsymbol{x}_i(t), \boldsymbol{x}_j(t - \tau_{ij}(t)), t),$$

$$\dot{\tau}_{ij} = h(\boldsymbol{x}_i(t), \boldsymbol{x}_j(t), t).$$

- Adaptive natural frequencies f_i
- With dynamical systems or with agent-based models
- Example: 'Hebbian' learning in coupled oscillators on networks
- It's often hard to make the models simple enough to do math.

Conclusions

- There are many different ways to generalize some approach or quantity (betweenness centrality, clustering coefficient, etc.) and many different choices to make in the process, so we need to think about which way to do it and what is most appropriate for a given problem.
- When generalizing, we lose some convenient feature (e.g., such as losing the guarantee that the leading eigenvalue and leading eigenvector are real) and then we need to figure out — through development of theory and/or methods — how to get the generalization to work.
- **"Springboarding from these discussions, we should try to set the stage for formulating interesting and concrete projects at the conclusion of the workshop."**