Multilayer Community Structure and Functional Brain Networks

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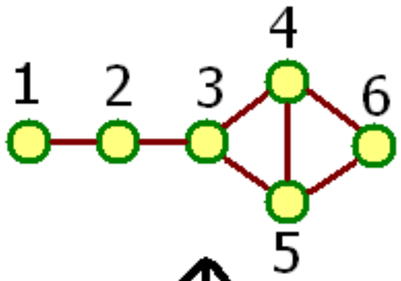
Some References (abridged)

- Review Articles on Multilayer Networks
  - Our article: M Kivelä, A. Arenas, M. Barthelemy, J. P. Gleeson, Y. Moreno, & MAP, "Multilayer Networks", *Journal of Complex Networks*, **2**(3): 203–271, 2014.
    - Tutorial slides: http://www.slideshare.net/masonporter/multilayer-tutorialnetsci2014slightlyupdated
  - Another review article: S. Boccaletti, G. Bianconi, et al., *Physics Reports*, 2014
- Expository Article on Community Structure
  - M. A. Porter, J.-P. Onnela, & P. J. Mucha, *Notices of the American Mathematical Society*, Vol. 56, No. 9: 1082–1097, 1164–1166 (2009)
    - Gives the state of play for community structure as of Oct. 2009. Very friendly introduction.
    - There is also a very long review article (S. Fortunato, *Physics Reports,* 2010).
- Methodology for Community Detection
  - P. J. Mucha, T. Richardson, Kevin Macon, M. A. Porter, & J.-P. Onnela, Science, Vol. 328, No. 5980, 876–878 (2010)
    - Introduces a method for multilayer community detection (for "multislice" type of multilayer networks)
    - We build on this in subsequent papers.
- Applications to Neuroscience
  - D. S. Bassett, N. F. Wymbs, M. A. Porter, P. J. Mucha, J. M. Carlson, & S. T. Grafton, PNAS, Vol. 118, No. 18, 7641–7646 (2011)
    - Numerous additional papers since this one
- Other Applications
  - Political voting networks, coupled nonlinear-oscillator models, financial assets, Lagrangian coherent structures, etc.
- Software
  - http://www.plexmath.eu/?page_id=327

Outline

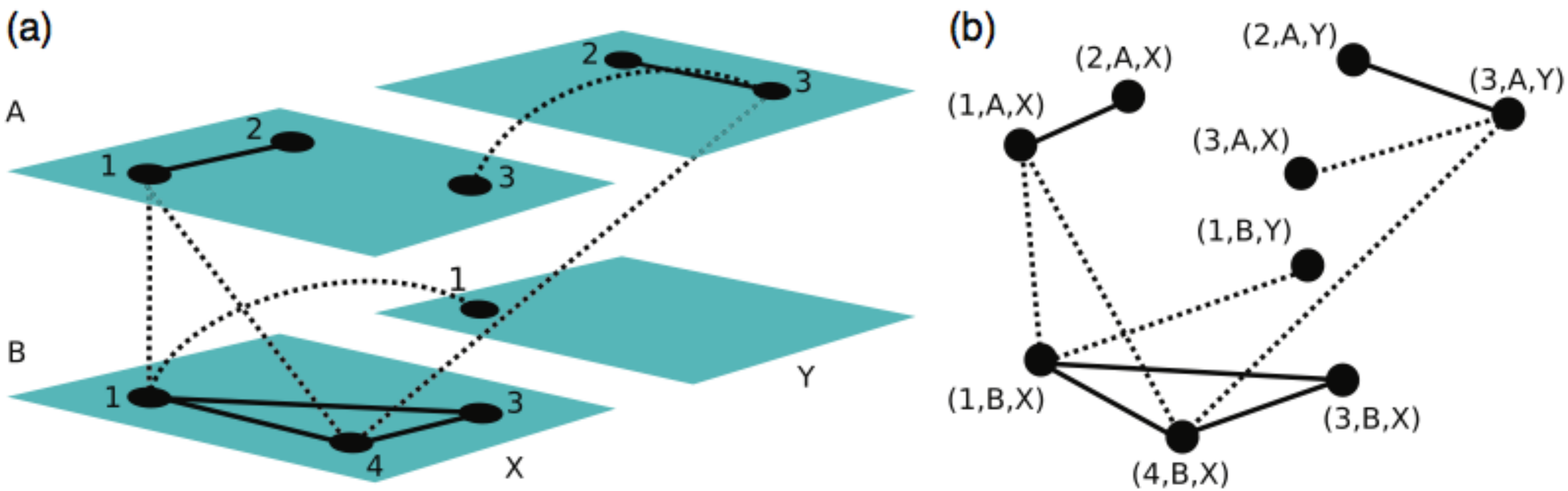
- What are *multilayer networks*?
- What is *community structure*?
- Community structure in multilayer networks
- Application to functional brain networks
  - "Flexibility" and motor learning
  - Community structure versus core-periphery structure
  - Cross-links (hypergraphs)
- Chunking in behavioral networks
- Developing null models for comparisons
- Conclusions and outlook

Network



$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix}$$

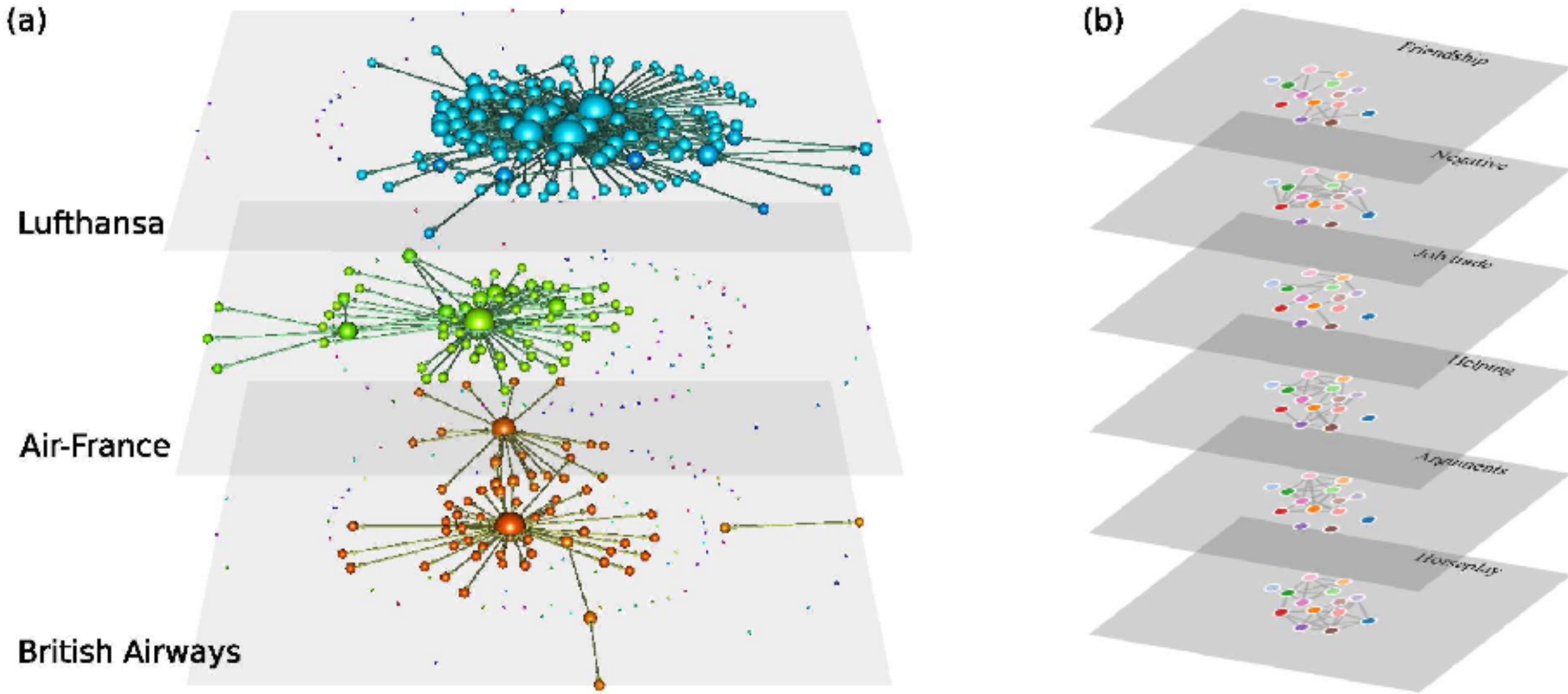
Multilayer Network




Multilayer-Network Gelatin Cake
Flora Meng

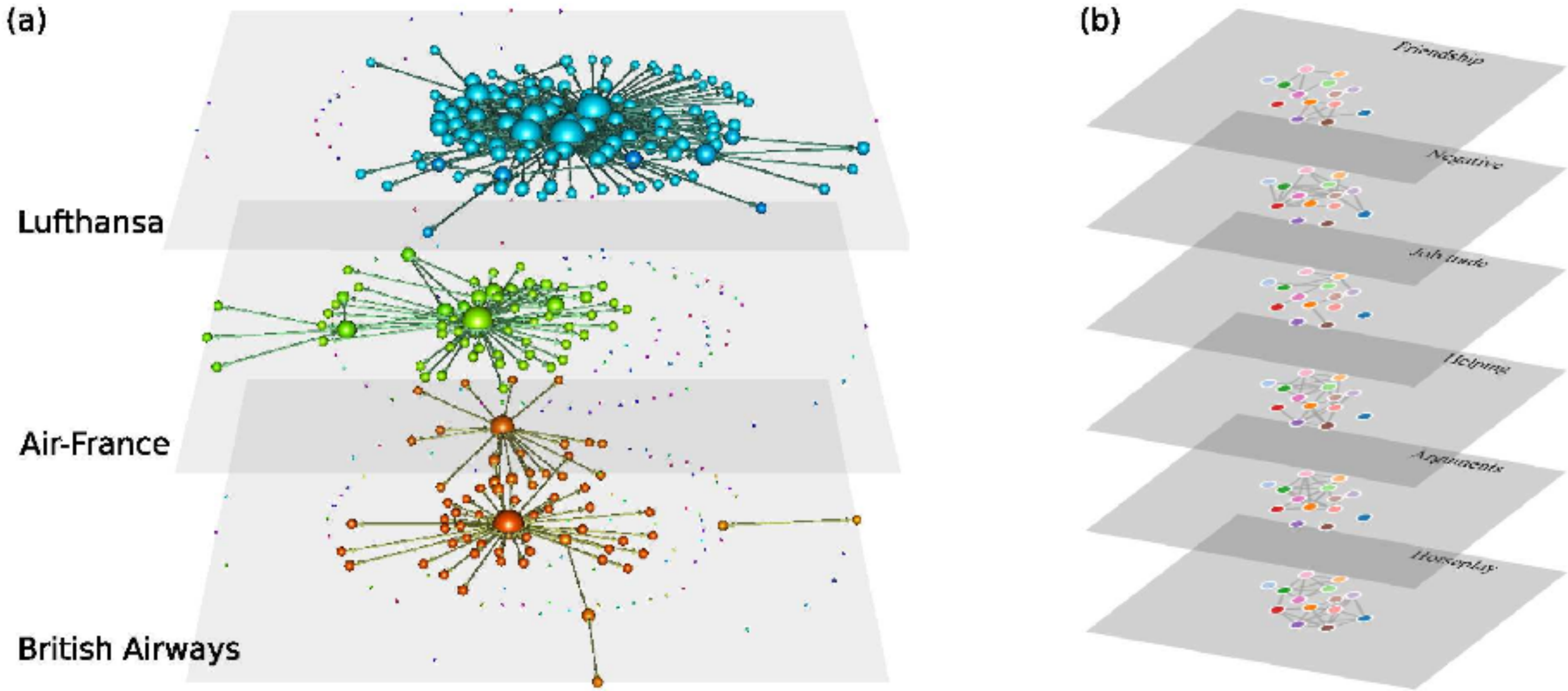
Example: Multiplex Network

- The concept of “multiplex network” has been around for many decades.



Software for Visualization and Analysis

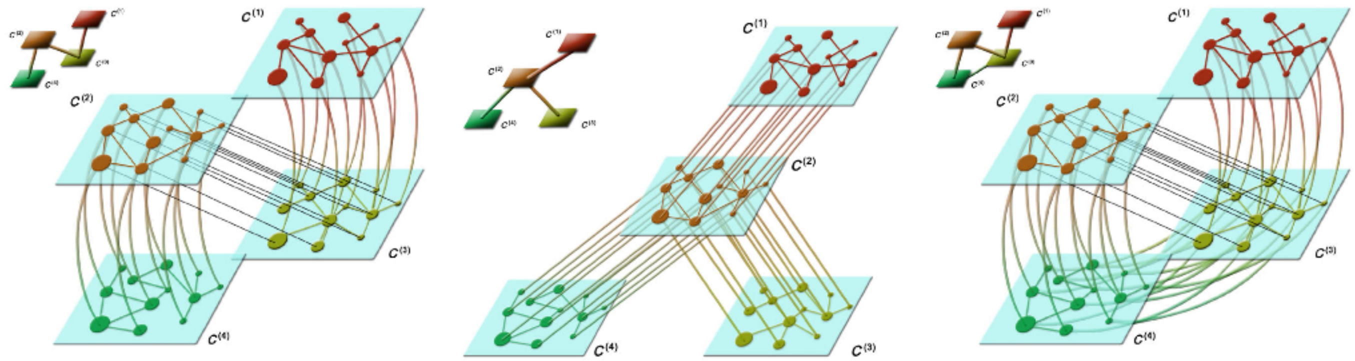
- See http://www.plexmath.eu/?page_id=327
- M. De Domenico, M. A. Porter, & A. Arenas, *Journal of Complex Networks*, advanced access: http://comnet.oxfordjournals.org/content/early/2014/10/12/comnet.cnu038.abstract



Example: Edge-Colored Multigraph

- Monster movement in the game "Munchkin Quest"

Example: Network of Networks



- The notion (and terminology) “network of networks” is also several decades old.

The City as a Network of Networks

To this point, we have been concerned primarily with ties between persons. There is nothing sacrosanct, however, about the assumption that network nodes must be individuals; network linkages may equally obtain between communities, between communities and more formally organized groups, between either of these and individuals, and so on. It is just as

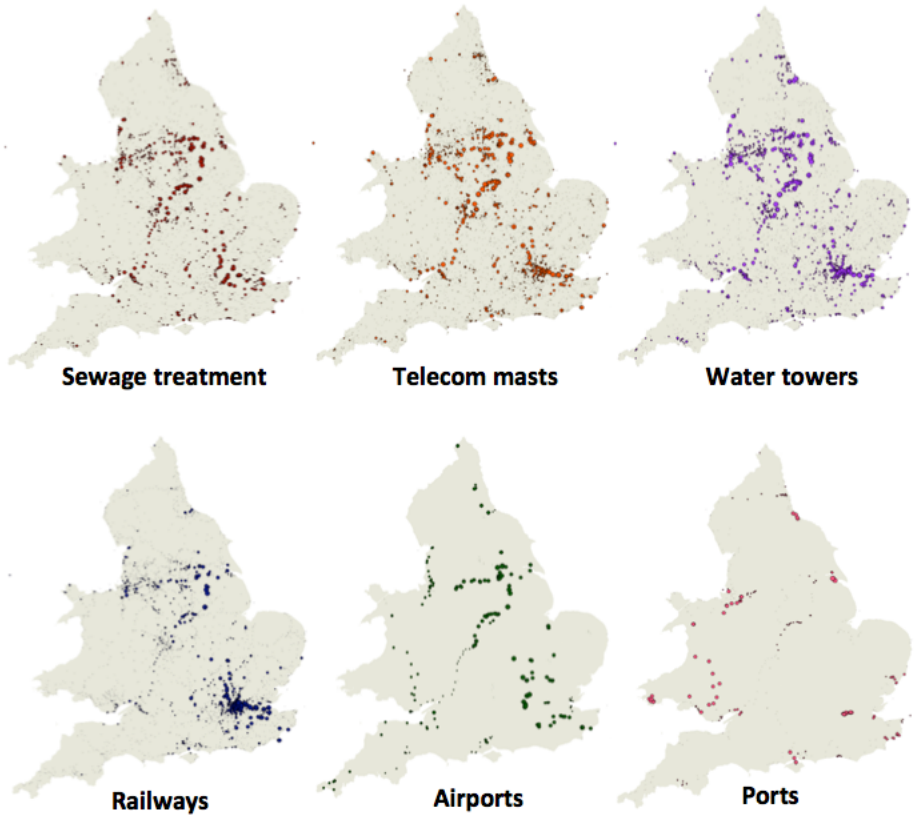
(Craven and Wellman, 1973)

A Network of Networks: UK Infrastructure

Direct customer demands
- Usage statistics where available
- Networks are more complicated..
    - Customer assignment models: – capacity constrained resource allocation model
    - Network effects

Electricity customers

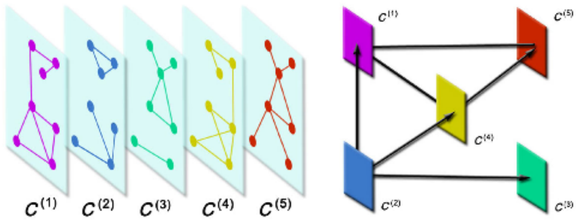
Indirect customer demands on Great Britain's electricity network



(Courtesy of Scott Thacker, ITRC, University of Oxford)

Multilayer Network

- Definition of a *multilayer network* M
  - $M = (V_M, E_M, V, L)$
    - V: set of nodes
      - As in ordinary graphs
    - L: sequence of sets of possible layers
      - One set for each additional "aspect" $d \geq 0$ beyond an ordinary network (examples: $d = 1$ in schematic on this page; $d = 2$ on last page)
    - V_M: set of tuples that represent *node-layers*
    - E_M: multilayer edge set that connects these tuples



- Note 1: allow weighted multilayer networks by mapping edges to real numbers with $w: E_M \rightarrow \boldsymbol{R}$
- Note 2: $d = 0$ yields the usual single-layer ("monoplex") networks

Tensorial Representation

- *Adjacency tensor* for unweighted case:

$$\mathcal{A} \in \{0,1\}^{|V|\times|V|\times|\mathbf{L}_1|\times|\mathbf{L}_1|\times\cdots\times|\mathbf{L}_d|\times|\mathbf{L}_d|}$$

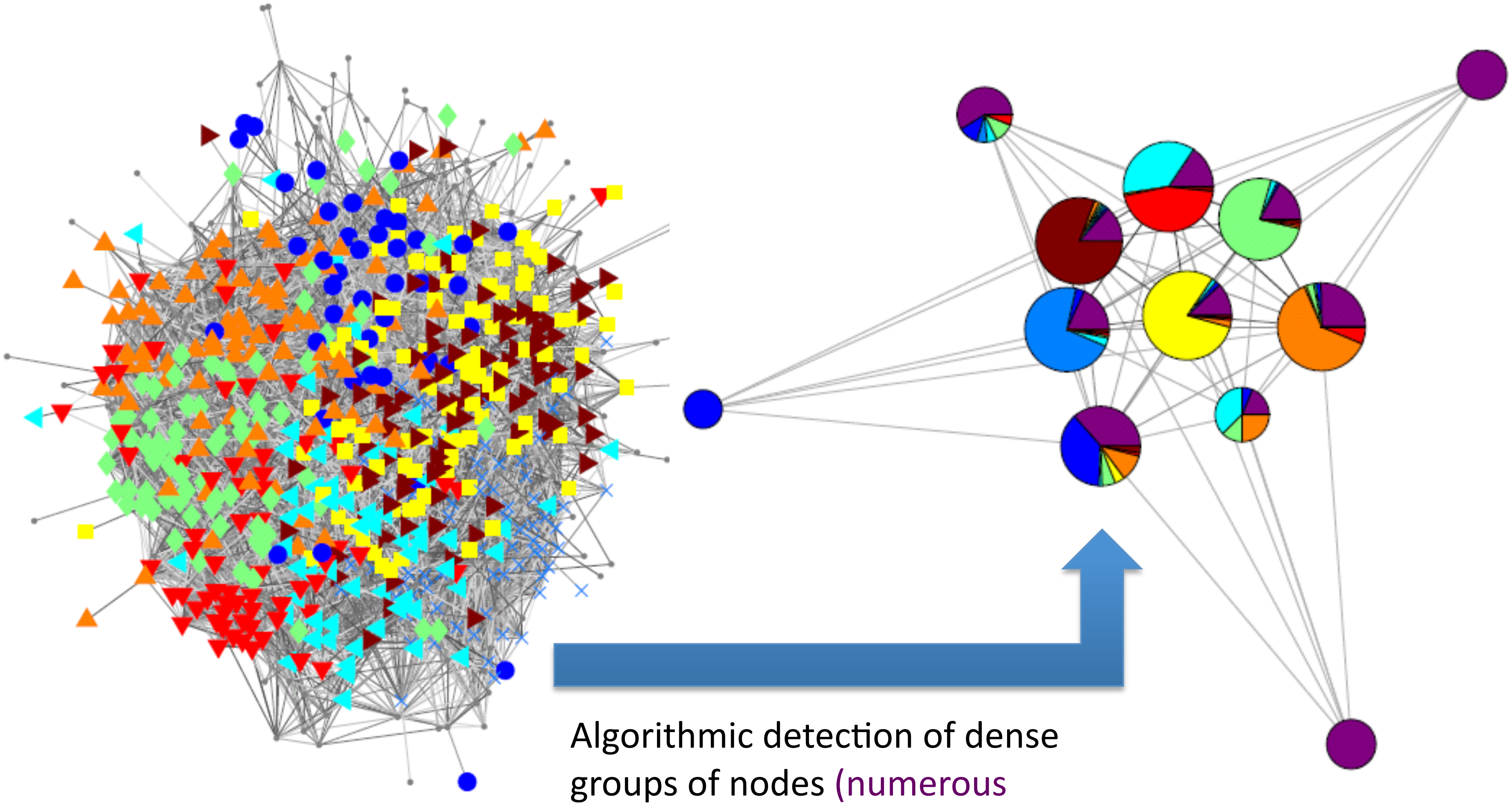
- Elements of adjacency tensor:
  - $A_{uv\boldsymbol{\alpha\beta}} = A_{uv\alpha 1\beta 1 \ldots \alpha d\beta d} = 1$ iff $((u,\boldsymbol{\alpha}), (v,\boldsymbol{\beta}))$ is an element of E_M (else $A_{uv\boldsymbol{\alpha\beta}} = 0$)

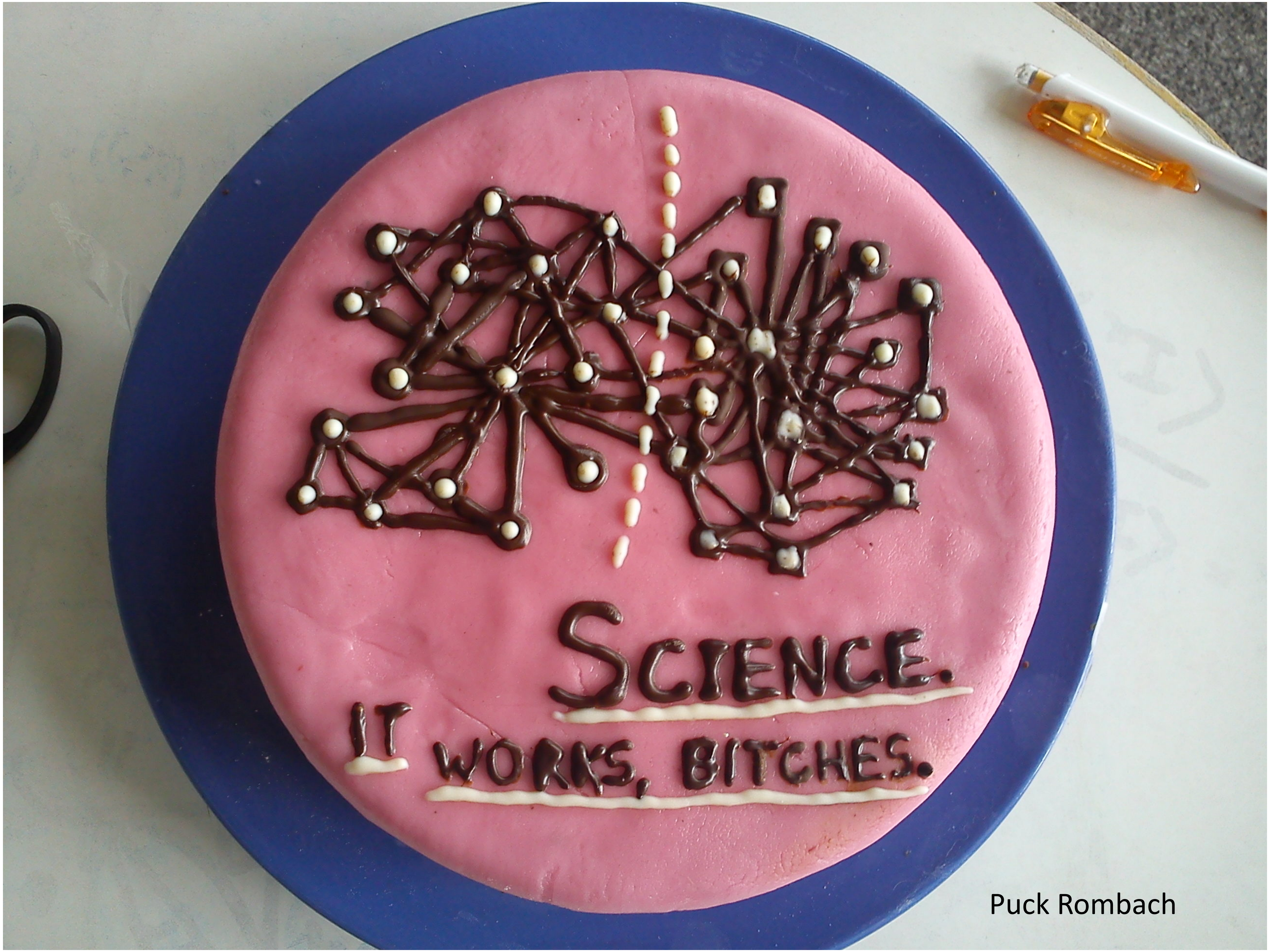
The literature is messy.

#makeitstop

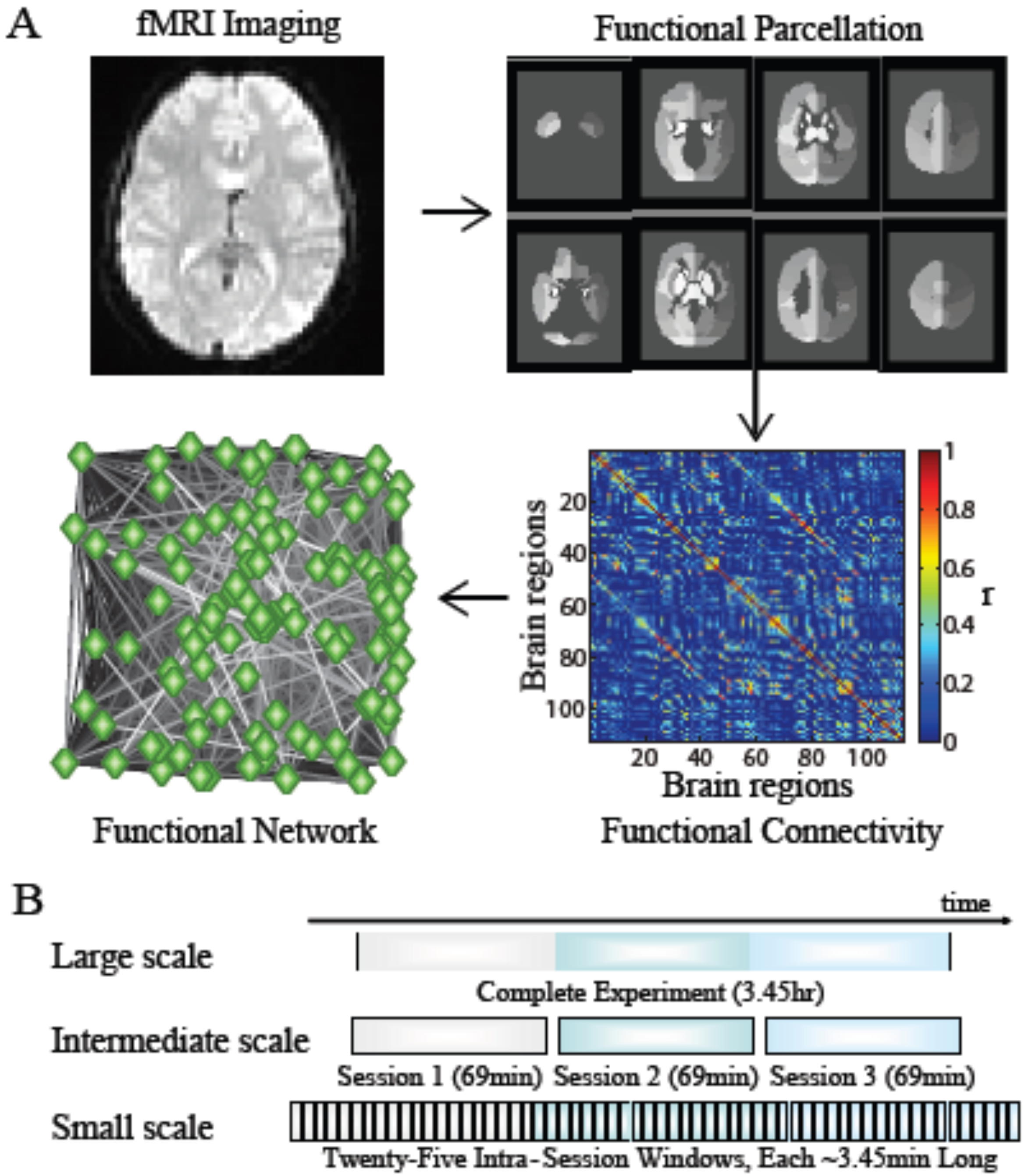
Name	Aligned	Disj.	Eq. Size	Diag.	Lcoup.	Cat.	$\|L\|$	d	Example refs.
Multilayer network				✓	✓	✓	Any	1	[58]
	✓†		✓†				Any	1	[79]
Multiplex network	✓†		✓†	✓			Any	1	[78, 79]
	✓		✓	✓	✓	✓	Any	1	[24, 34, 49, 62, 125, 198, 287]
	✓		✓	✓	✓	✓	2	1	[154, 180, 182]
				✓	✓	✓	Any	1	[70]
	✓		✓	✓	✓		Any	1	[71, 242, 243]
Multivariate network	✓		✓	✓	✓	✓	Any	1	[209]
Multinetwork	✓		✓	✓	✓	✓	Any	1	[14]
	✓		✓	✓	✓	✓	Any	2	[15]
Multirelational network	✓		✓	✓	✓	✓	Any	1	[55, 119, 252, 278]
Multirelational data	✓		✓	✓	✓	✓	Any	1	[160, 197]
Multilayered network	✓		✓	✓	✓	✓	Any	1	[45–47, 242]
Multidimensional network	✓		✓	✓	✓	✓	Any	1	[18, 31–33, 69, 140, 264]
	✓		✓	✓	✓	✓	Any	3	[141]
Multislice network	✓†		✓†	✓			Any	1	[22, 56, 187, 188]
Multiplex of interdep. networks	✓		✓	✓	✓	✓	Any	1	[111]
Hypernetwork	✓		✓	✓	✓	✓	Any	1	[131, 247]
Overlay network	✓		✓	✓	✓	✓	2	1	[97, 170]
Composite network	✓		✓	✓	✓	✓	2	1	[282]
Multilevel network				✓	✓	✓	Any	1	[70, 74]
**		✓					Any	1	[153, 272]
Multiweighted graph	✓		✓	✓	✓	✓	Any	1	[218]
Heterogeneous network		✓					2	1	[55, 294]
Multitype network		✓					Any	1	[8, 120, 269]
Interconnected networks		✓	✓				2	1	[81, 164]
		✓					2	1	[225, 229]
Interdependent networks*			✓				Any	1	[244]
			✓				2	1	[173]
		✓					2	1	[48, 110]
	✓		✓	✓	✓	✓	Any	1	[25]
Partially interdep. networks*			✓				2	1	[244]
Network of networks*			✓				Any	1	[98]
Coupled networks				✓	✓	✓	Any	1	[288]
Interconnecting networks				✓	✓	✓	2	1	[286]
Interacting networks		✓					Any	1	[85, 155]
		✓					2	1	[48]
Heterogenous information net		✓					Any	1	[258]
**							Any	2	[77, 255–257]
Meta-matrix, meta-network							Any	2	[60, 61, 266]

Community Detection

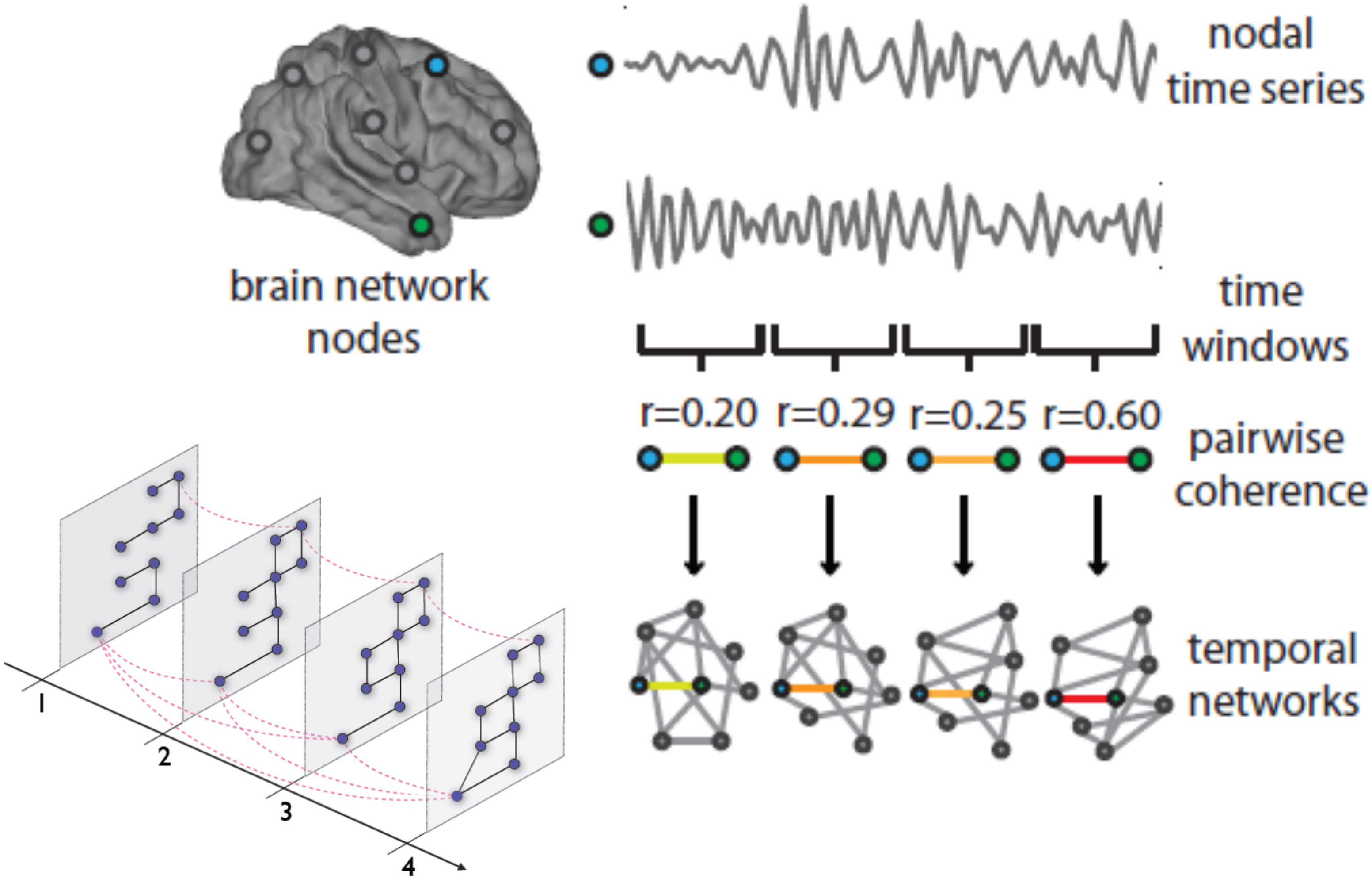




Puck Rombach


A
fMRI Imaging
Functional Parcellation
Brain regions
20
40
60
80
100
20
40
60
80
100
Brain regions
1
0.8
0.6
0.4
0.2
0
r
Functional Network
Functional Connectivity
B
time
Large scale
Complete Experiment (3.45hr)
Intermediate scale
Session 1 (69min)
Session 2 (69min)
Session 3 (69min)
Small scale
Twenty-Five Intra-Session Windows, Each ~3.45min Long

Time-Dependent Networks (e.g. from fMRI data): Multilayer Representation

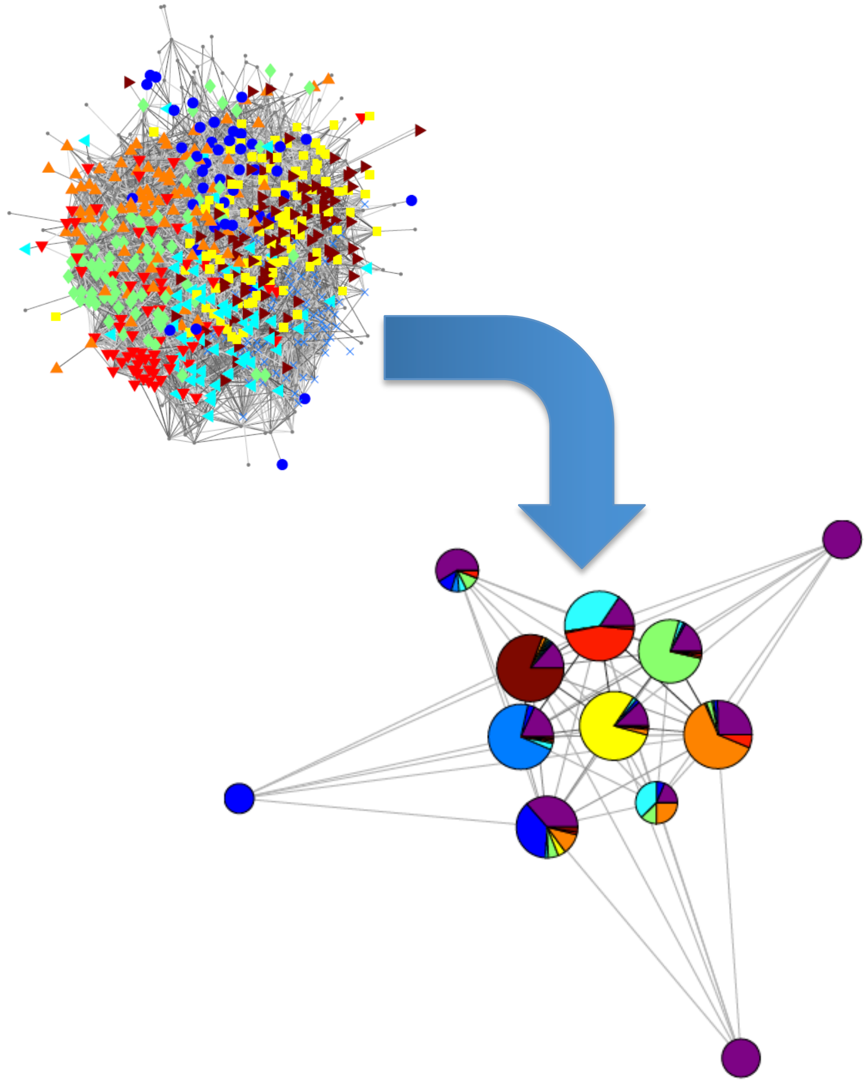


Community Structure

- "Hard/rigid" versus "soft/fuzzy/overlapping" clustering
- A *community* should describe a "cohesive group" of nodes
  - Tons of algorithms available
- Usual notion: more intra-community edges than one would expect at random
  - *But what does "at random" mean?*
- Review articles
  - "Communities in Networks," M. A. Porter, J.-P. Onnela & P. J. Mucha, *Notices of the American Mathematical Society* **56**, 1082–1097 & 1164–1166 (2009).
  - "Community Detection in Graphs," S. Fortunato, *Physics Reports* **486**, 75–174 (2010).

Network Communities

- Communities = cohesive groups/modules/ mesoscopic structures
  - In stat phys, you try to derive macroscopic and mesoscopic insights from microscopic information
- Community structure consists of complicated interactions between modular (horizontal) and hierarchical (vertical) structures
- Communities have denser set of internal links relative to some null model for what links are present at random
  - "Modularity"



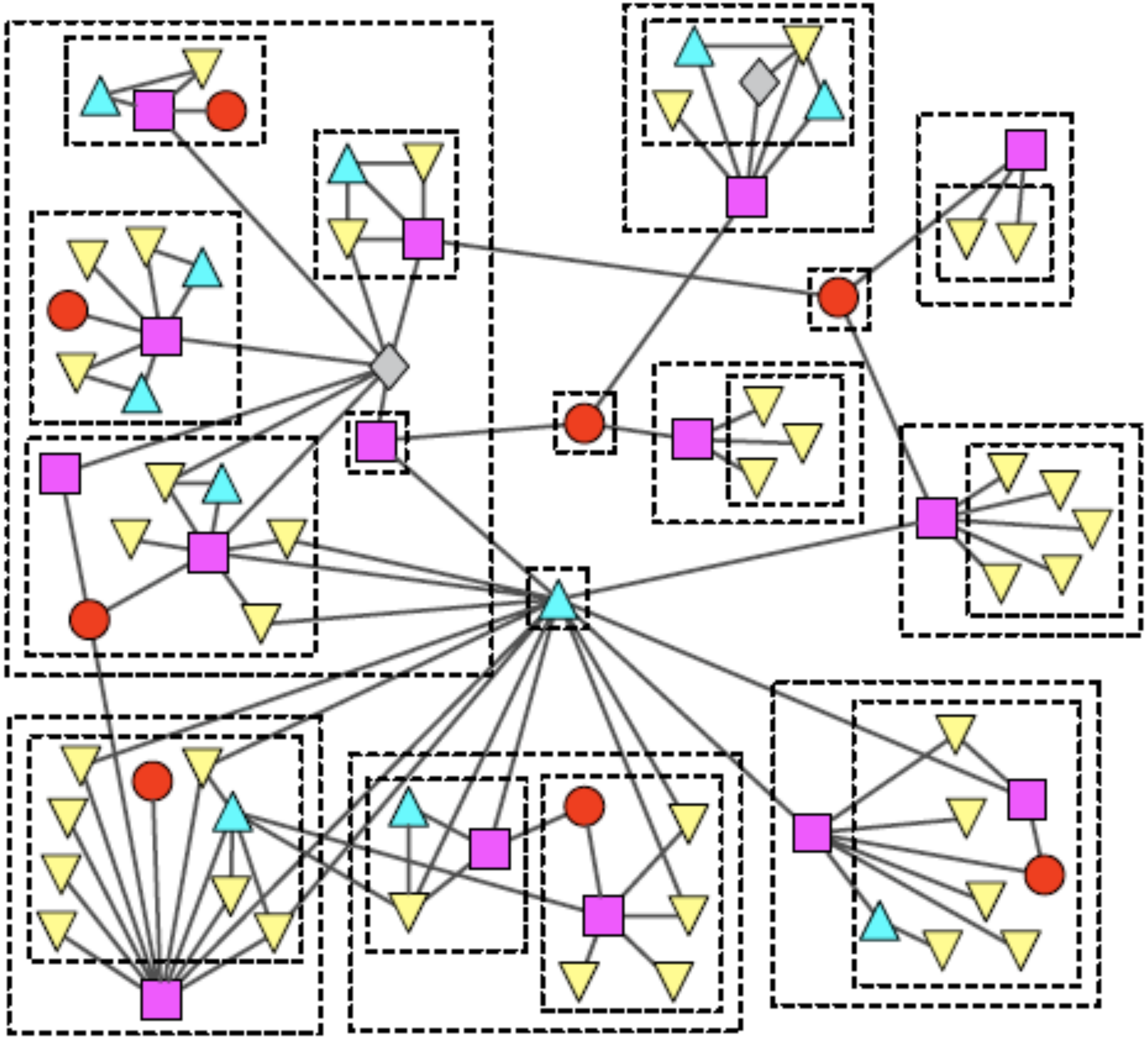


Image from A. Clauset, C. Moore, & M. E. J. Newman (*Nature*, 2008)

Quality / Modularity

- Popular approach: Use a "modularity" quality function

$$Q = \frac{1}{2W}\sum_{i,j} B_{ij}\delta(C_i, C_j)\,, \quad B_{ij} = A_{ij} - P_{ij}$$

where $\delta(C_i, C_j)$ indicates that the B_{ij} components are only summed over cases in which nodes i and j are classified in the same community. The factor $W = \frac{1}{2}\sum_{ij} A_{ij}$ is the total edge strength in the network (equal to the total number of edges for unweighted networks), where k_i again denotes the strength of node i. In (3.2), P_{ij} denotes the components of a *null model* matrix, which specifies the relative value of intra-community edges in assessing when communities are closely connected [8, 77].

- GOAL: Assign nodes to communities to maximize Q.

Example Null Models

(aka: what does "at random" mean?)

- Erdös-Rényi (Bernoulli)

$$P_{ij} = p$$

- Newman-Girvan*

$$P_{ij} = \gamma \frac{k_i k_j}{2W}$$

- Leicht-Newman* (directed)

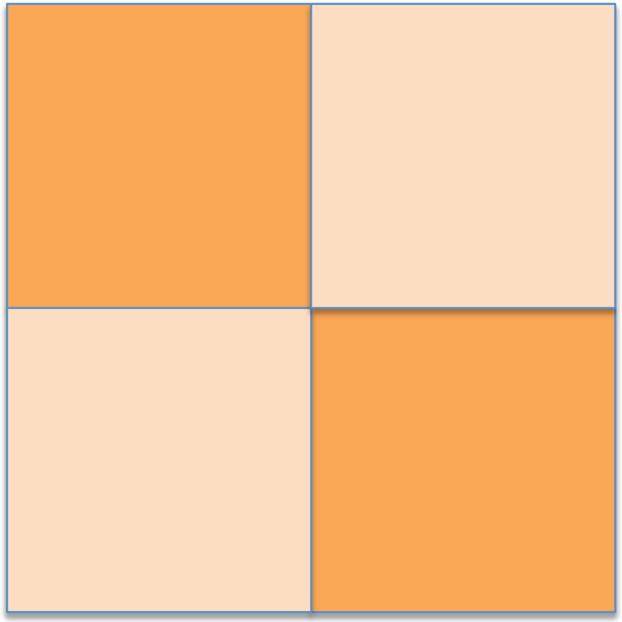
$$P_{ij} = \gamma \frac{k_i^{in} k_j^{out}}{W}$$

- Barber* (bipartite)

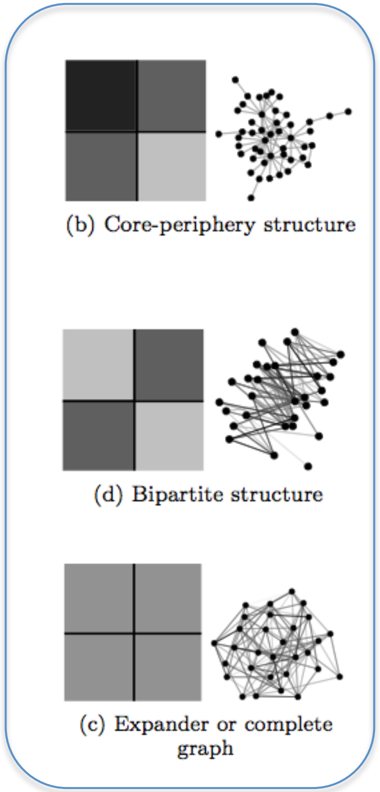
$$P_{ij} = \begin{cases} \gamma \frac{k_i d_j}{W} \\ 0 \end{cases}$$

** With additional resolution parameter γ*

Platonic ideal of block structure for "traditional" Newman-Girvan choice of Q (nested version of this)



Community Structure

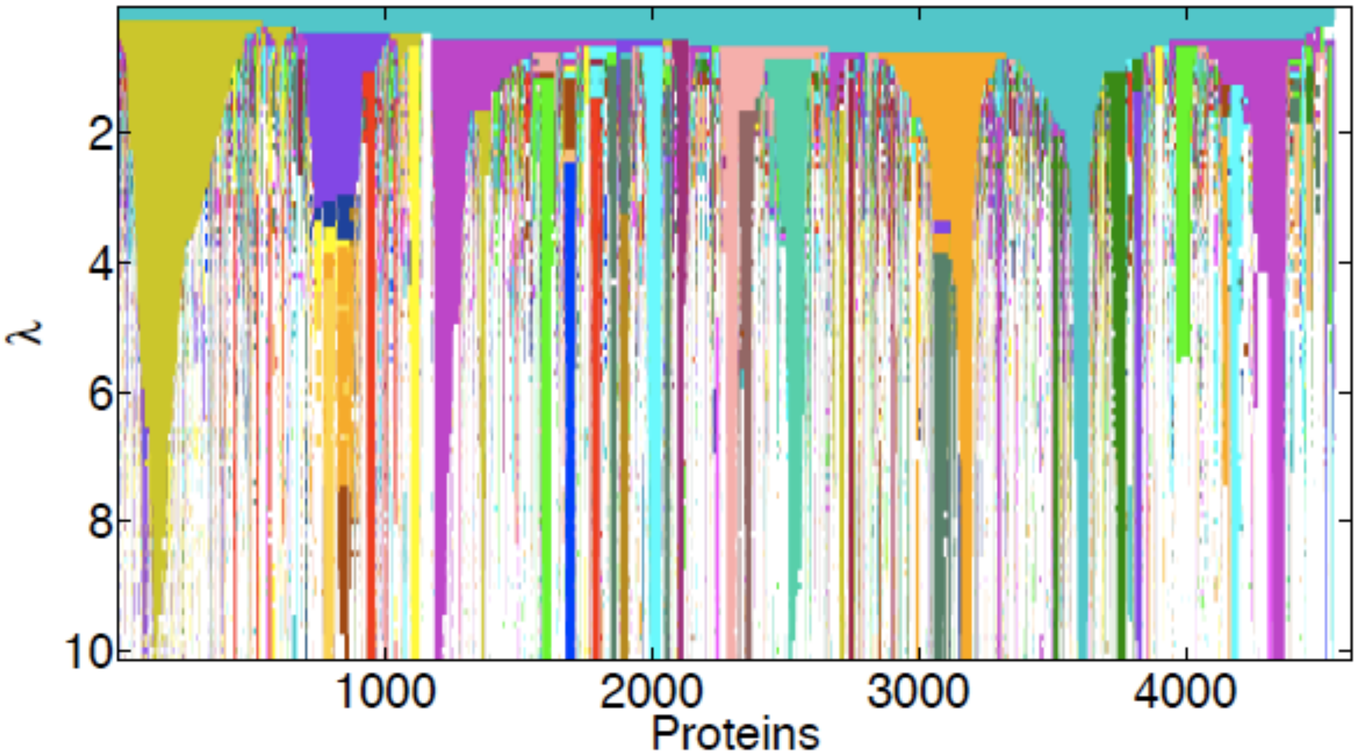


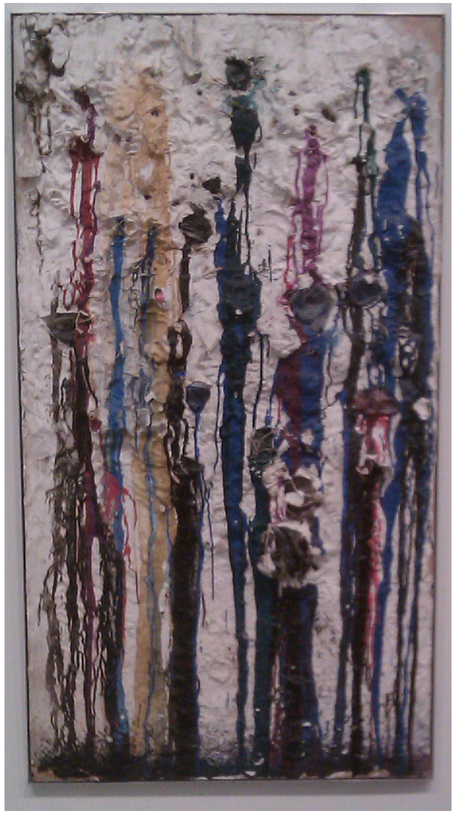
- This can be generalized, though the vast majority of methods have this in mind…
    - Note: I will focus on hard partitioning, but one can also think about overlapping communities in multilayer networks.

Real Networks: Onion Peeling

Example: Protein-Protein Interaction Networks

A. C. F. Lewis, N. S. Jones, MAP, & C. M. Deane, *BMC Systems Biology* **4**: 100 (2010)



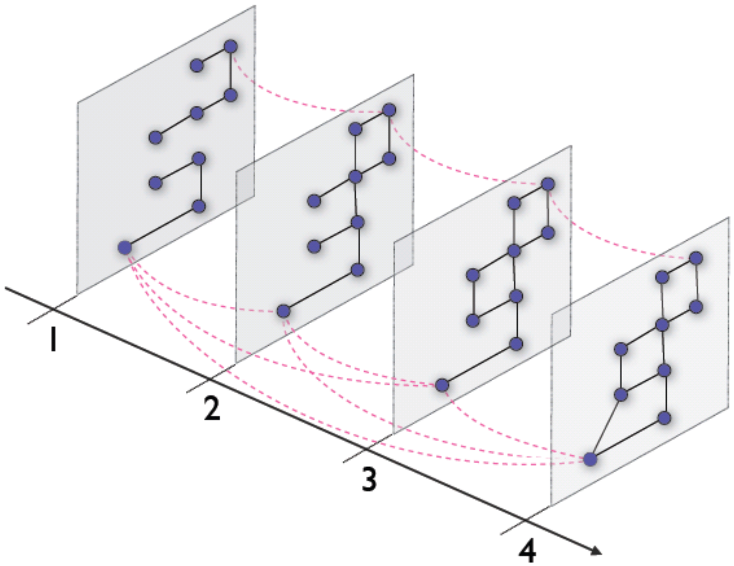


Community Detection: Computational Heuristics

$$Q = \frac{1}{2W} \sum_{i,j} B_{ij} \delta(C_i, C_j)\,, \;\; B_{ij} = A_{ij} - P_{ij}$$

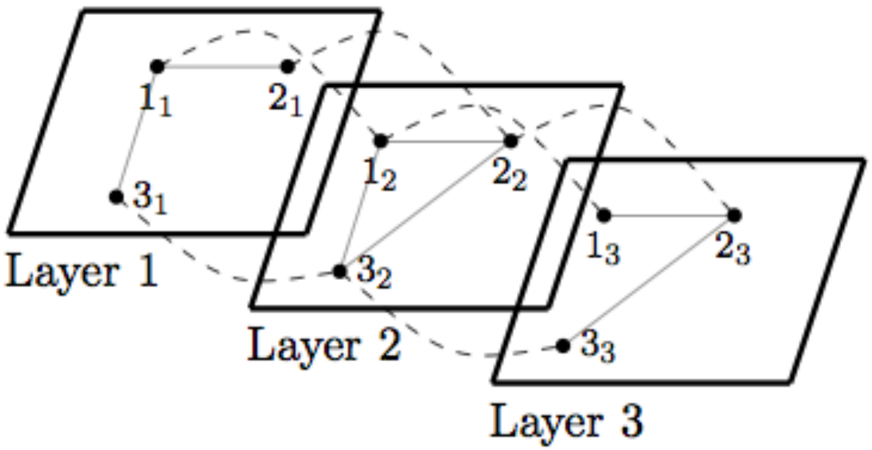
- Cannot guarantee optimal quality without full enumeration of possible partitions
  - NP-hard problem
  - Many algorithms available (spectral, Louvain, etc.)
  - Need to pick null model appropriate to problem
  - Extreme near-degeneracies in "good" local optima of Q
    - (B. H. Good, Y.-A. de Montjoye, & A. Clauset, *PRE*, 2010)

"Multislice" Networks (Mucha et al, 2010)
[a type of multilayer network]



- Traditional formulation for studying networks: Static networks with a single kind of edge and partitioned at a single spatial resolution
  - Also potentially sweep over multiple resolutions (or over multiple static snapshots) but in an ad hoc fashion
- Multislice framework: time-dependent, multiplex, and with communities at multiple scales
- Simple idea: Glue common brain regions across "slices" (i.e. "layers")

2.3 "Flattened" Multislice Networks (supra-adjacency representation)



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

- Schematic from M. Bazzi, MAP, S. Williams, M. McDonald, D. J. Fenn, & S. D. Howison, in preparation

What is an appropriate null model?

$$Q = \frac{1}{2W} \sum_{i,j} B_{ij} \delta(C_i, C_j)\,, \;\; B_{ij} = A_{ij} - P_{ij}$$

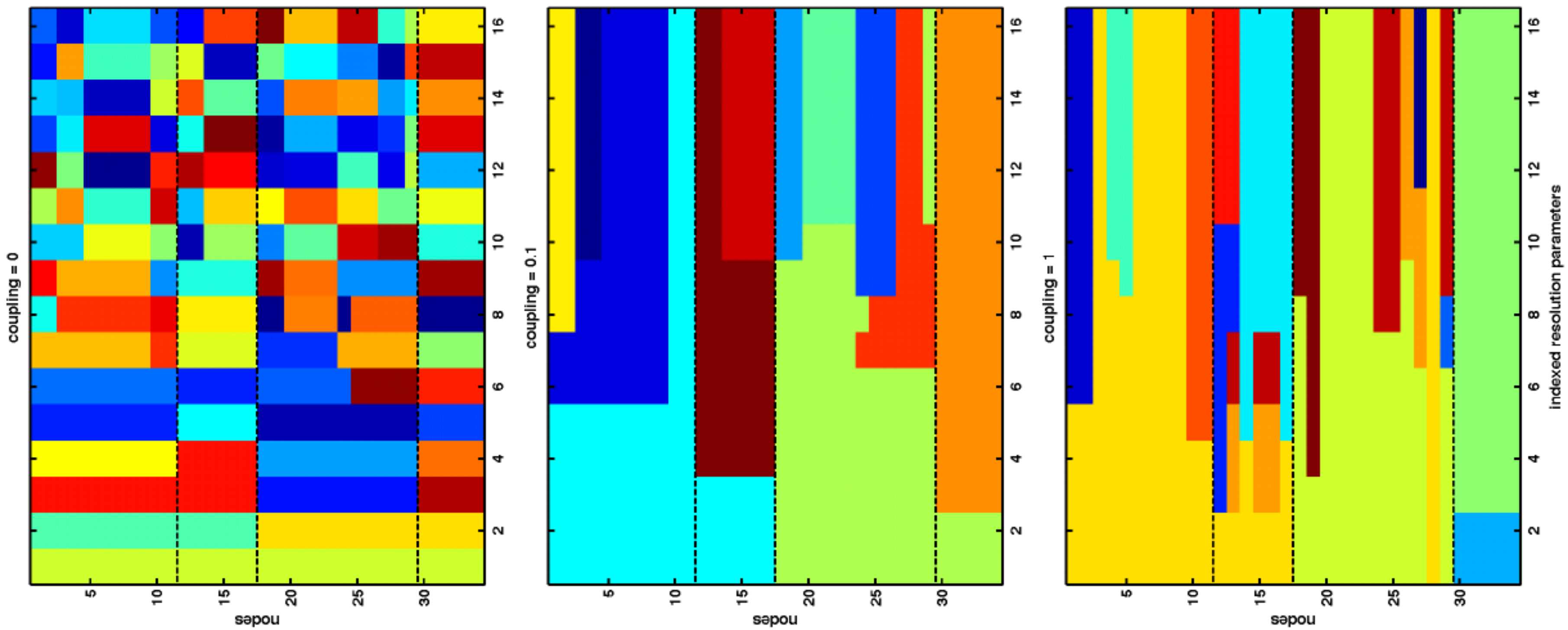
- Each layer is a network (static, single type of edge) with a specified spatial resolution of interest
- Different layers can mean: different value of resolution parameter, different time snapshot, different type of connection
- Have both intra-layer edges & inter-layer edges
- How to choose a null model?

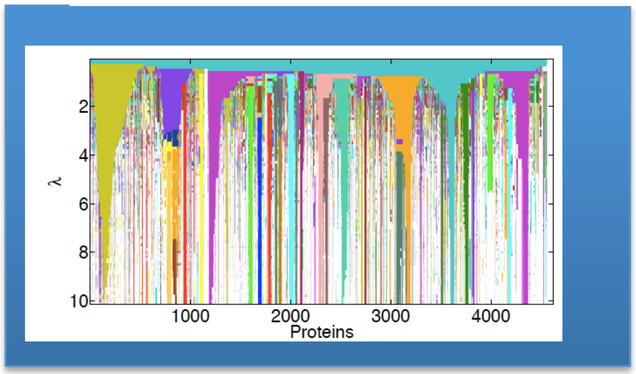
Multislice Modularity

- Find communities algorithmically by optimizing "multislice modularity"
  - We derived this function in Mucha et al, 2010
    - Laplacian dynamics: find communities based on how long random walkers are trapped there. Exponentiate and then linearize to derive modularity.
    - Generalizes derivation of ordinary modularity from R. Lambiotte, J.-C. Delvenne, &. M Barahona, arXiv:0812.1770
  - Brain region *x* in layer *r* is a *different node* from brain region *x* in layer *s*
    - A *layer* could come from e.g. similarities between regions computed during some time window

$$Q_{\text{multislice}} = \frac{1}{2\mu} \sum_{ijsr} \left\{ \left(A_{ijs} - \gamma_s \frac{k_{is} k_{js}}{2m_s} \right) \delta_{sr} + \delta_{ij} C_{jsr} \right\} \delta(g_{is}, g_{jr})$$

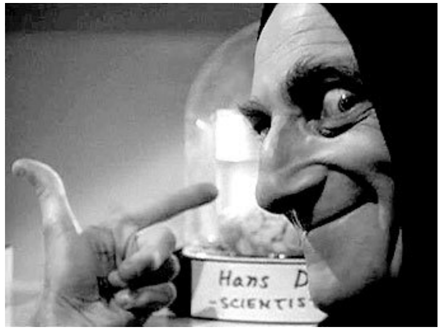
Example: Zachary Karate Club

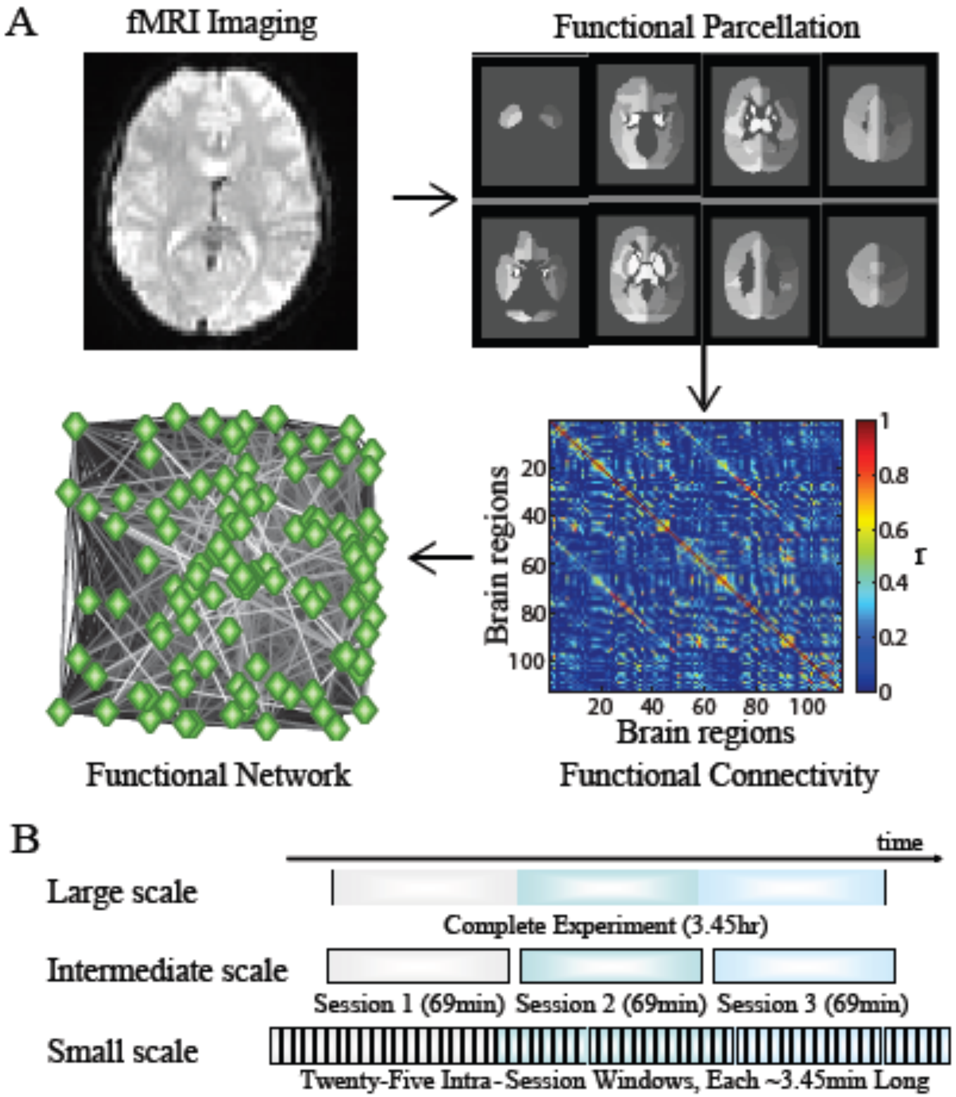


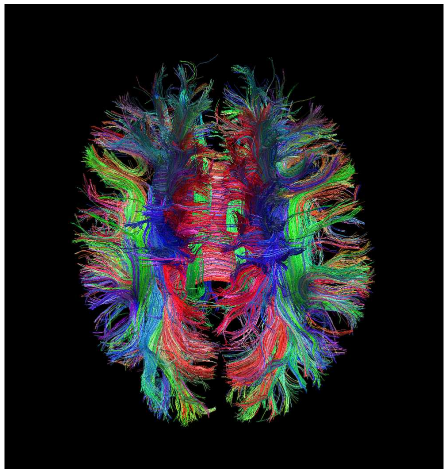


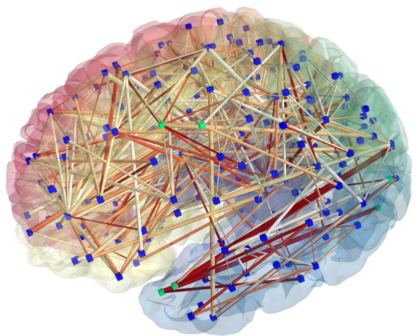
$$C_{jsr} = \{0, \omega\}$$

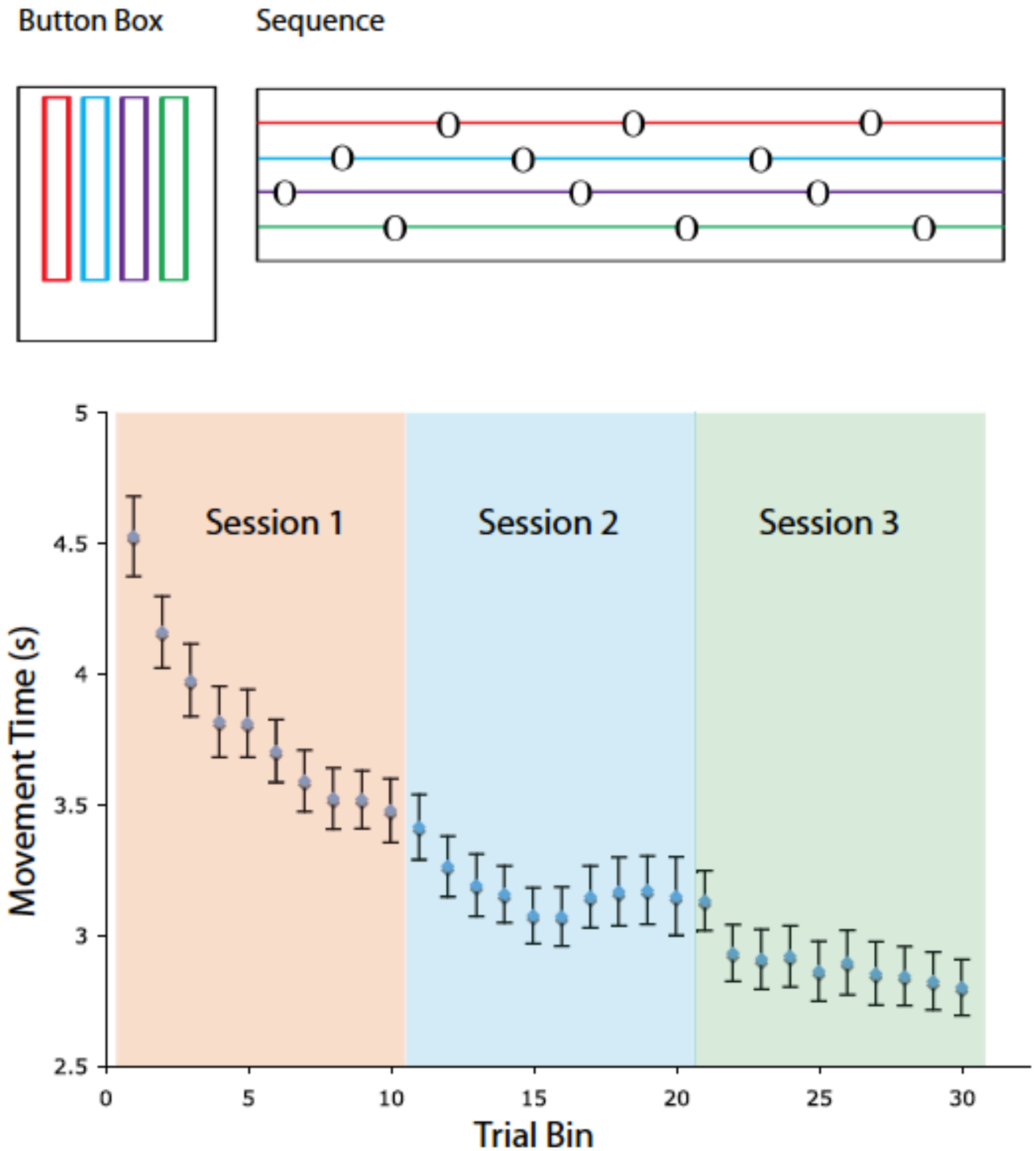
Braiiiiiiiiiiiiins





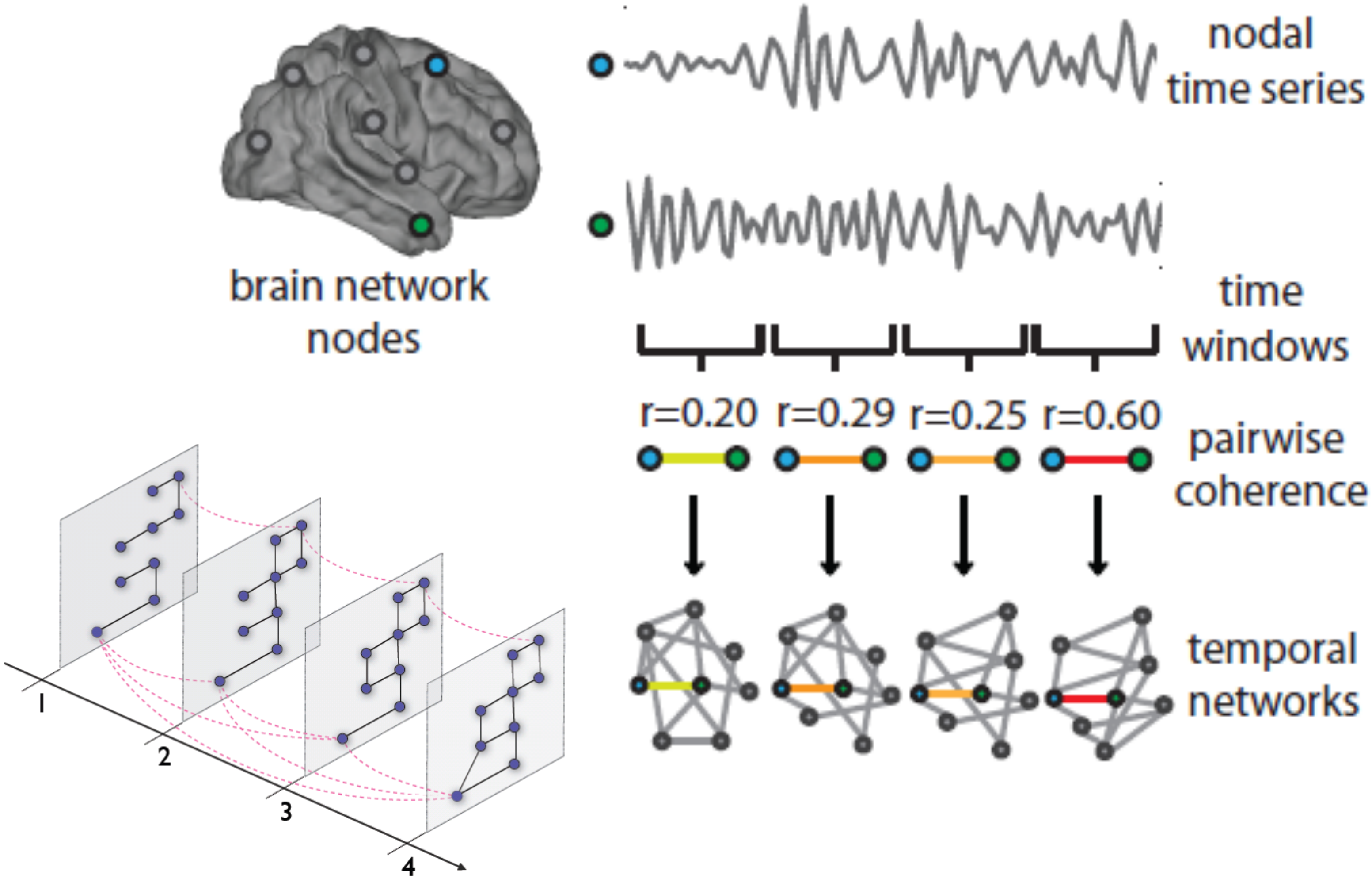






Button Box
Sequence
Session 1
Session 2
Session 3
Movement Time (s)
Trial Bin
5
4.5
4
3.5
3
2.5
0
5
10
15
20
25
30

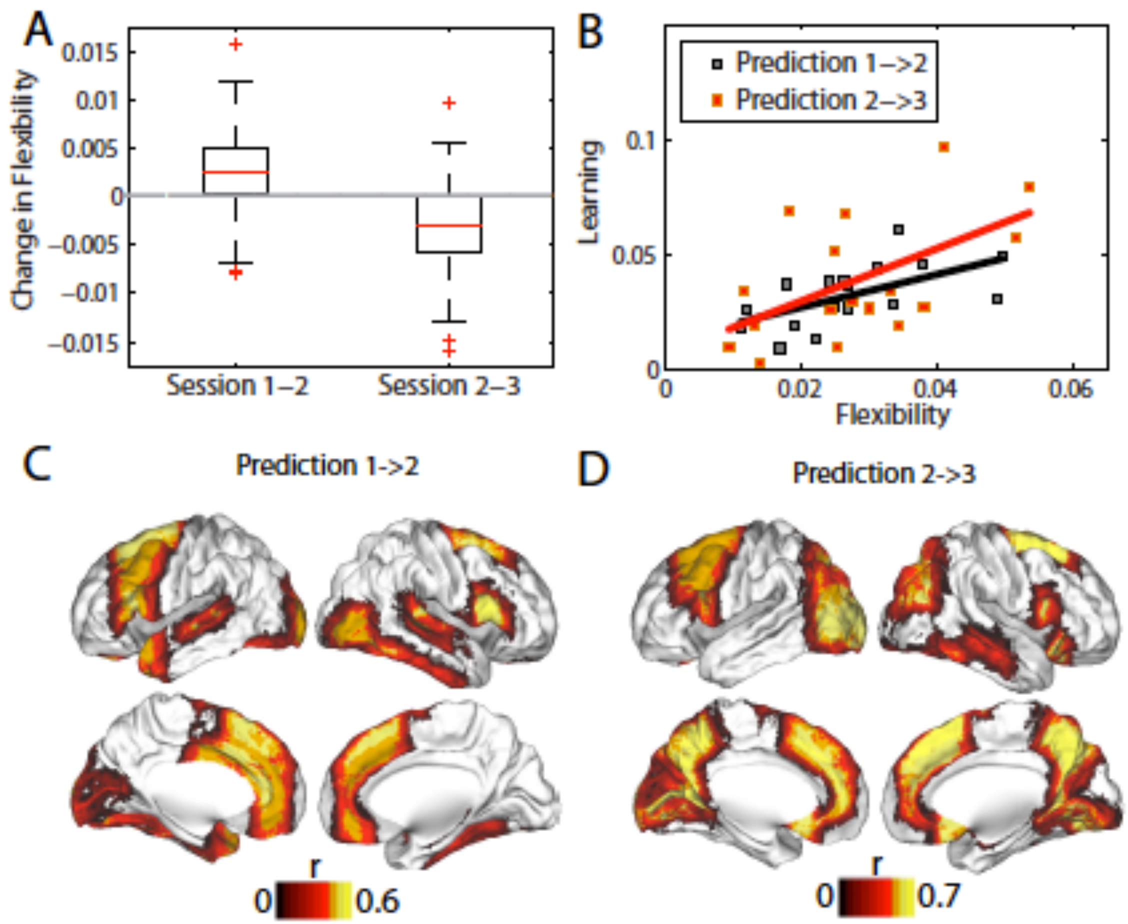
Constructing Time-Dependent Networks



Dynamic Reconfiguration of Human Brain Networks During Learning

(Bassett et al, *PNAS*, 2011)

- fMRI data: network from correlated time series
- Examine role of modularity in human learning by identifying dynamic changes in modular organization over multiple time scales
- Main result: flexibility, as measured by allegiance of nodes to communities, in one session predicts amount of learning in subsequent session



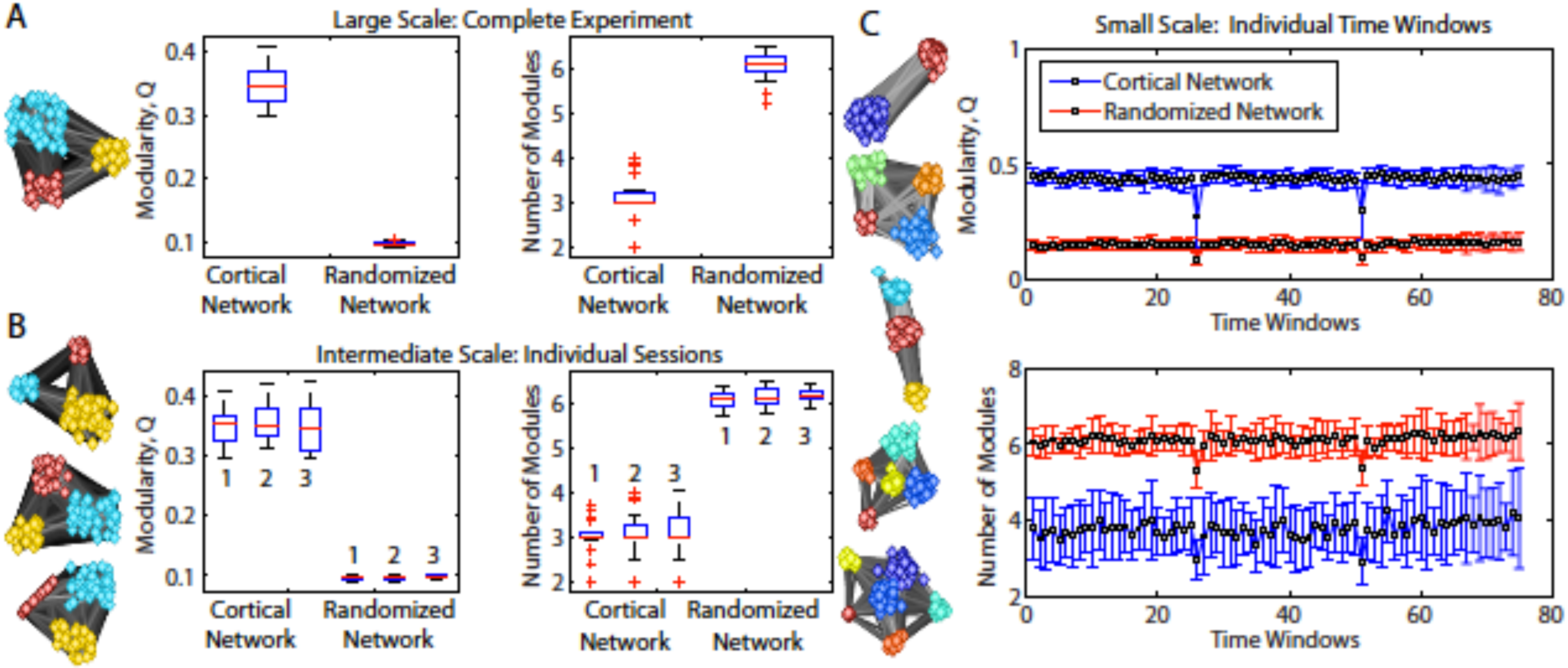
Stationarity and Flexibility

- Community stationarity ζ (autocorrelation over time of community membership):

$$U(t, t+m) \equiv \frac{|G(t) \cap G(t+m)|}{|G(t) \cup G(t+m)|} \qquad \zeta \equiv \frac{\sum_{t=t_0}^{t'-1} U(t, t+1)}{t' - t_0 - 1}$$

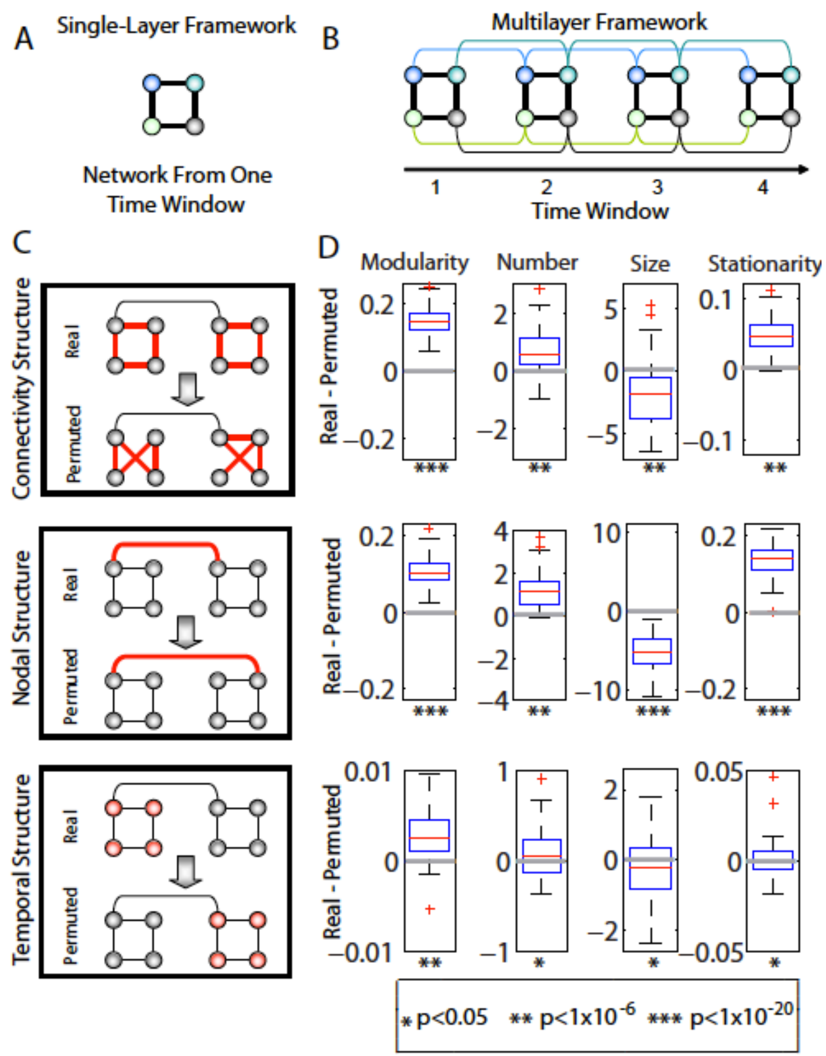
- Node flexibility:
  - f_i = number of times node i changed communities divided by total number of possible changes
  - Flexibility $f = \langle f_i \rangle$

Time Evolution of Static Communities



Dynamic Community Structure

- Investigating community structure in a multilayer framework requires consideration of new null models
- Many more details!
  - E.g., Robustness of results to choice of size of time window, size of inter-slice coupling, particular definition of flexibility, complicated modularity landscape, definition of 'similarity' of time series, etc.



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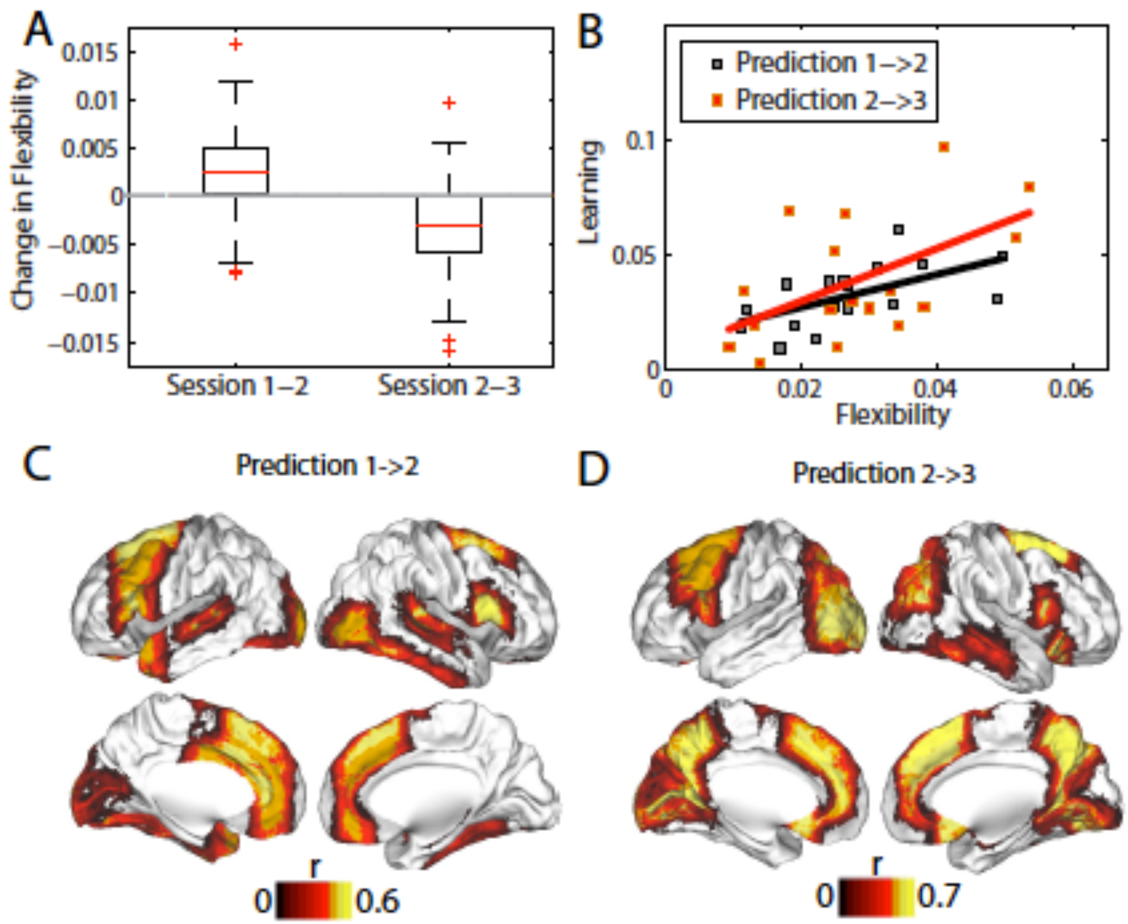
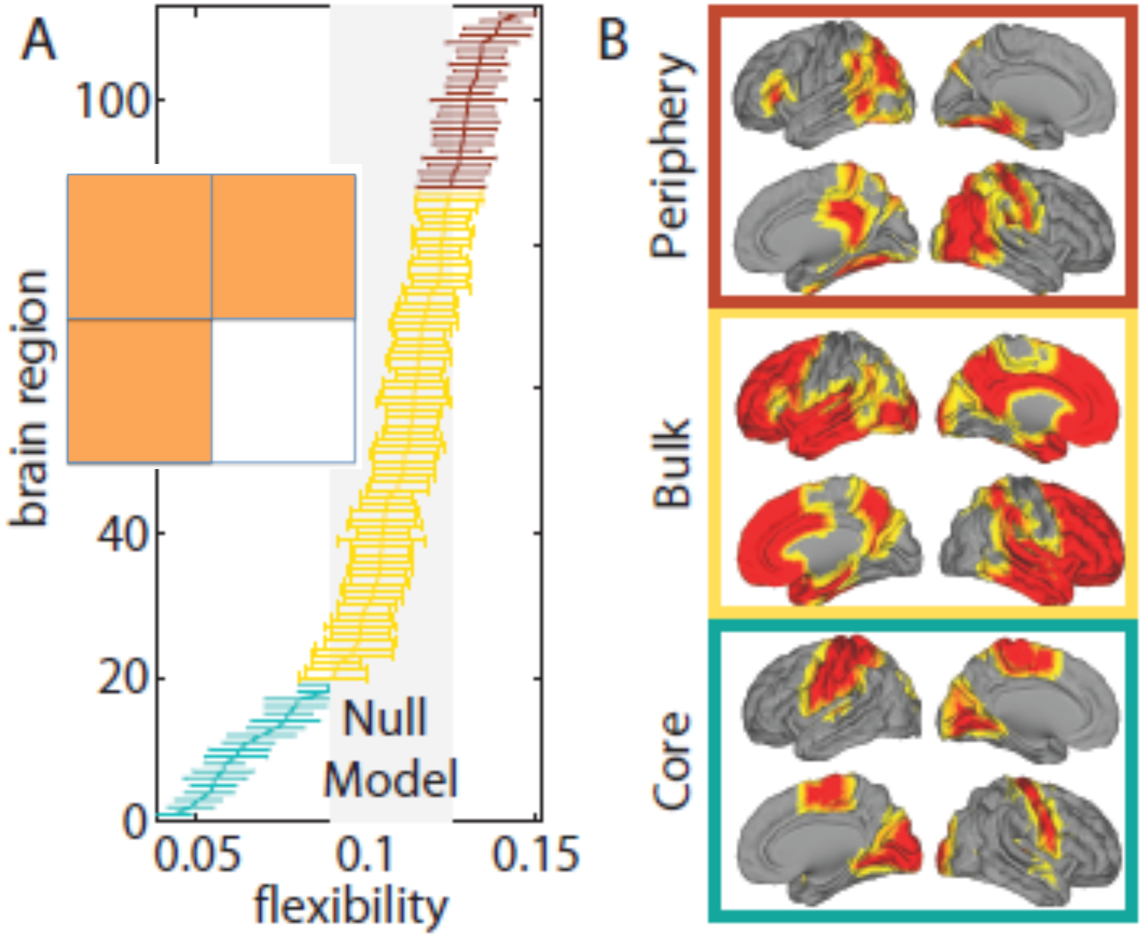
- Examine role of modularity in human learning by identifying dynamic changes in modular organization over multiple time scales
- Main result: flexibility, as measured by allegiance of nodes to communities, in one session predicts amount of learning in subsequent session

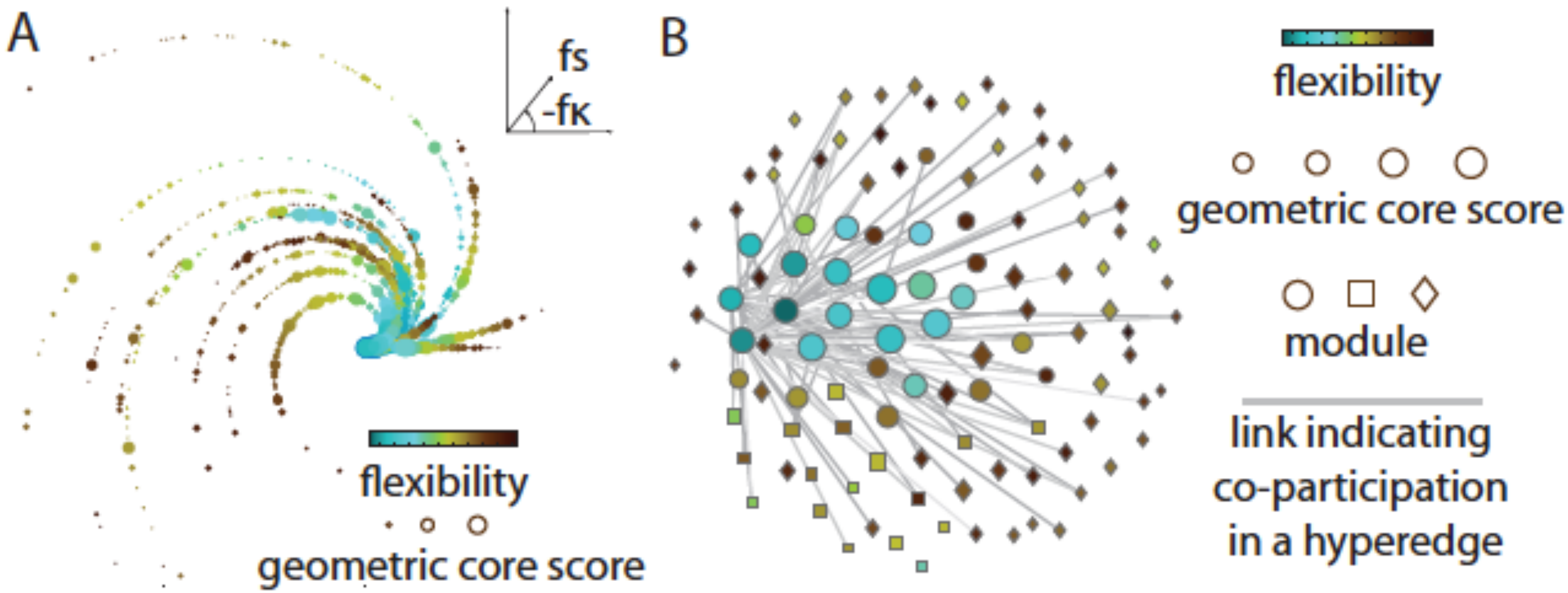


Which Brain Regions are "Flexible"?

- D. S. Bassett, N. F. Wymbs, M. P. Rombach, MAP, P. J. Mucha, & S. T. Grafton, *PLoS Comp. Bio.* **9**(9): 1003171 (2013)
- Flexible nodes are consistently in a "periphery" as computed for static networks encompassing given time windows
- Nodes that are not flexible (call them "stiff") are consistently in a structural core in these static networks
- Note: I have not discussed our methodology for computing core-periphery structure
  - M. P. Rombach, MAP, J. H. Fowler, & P. J. Mucha, *SIAM J. App. Math.* **74**(1): 167–190 (2014)



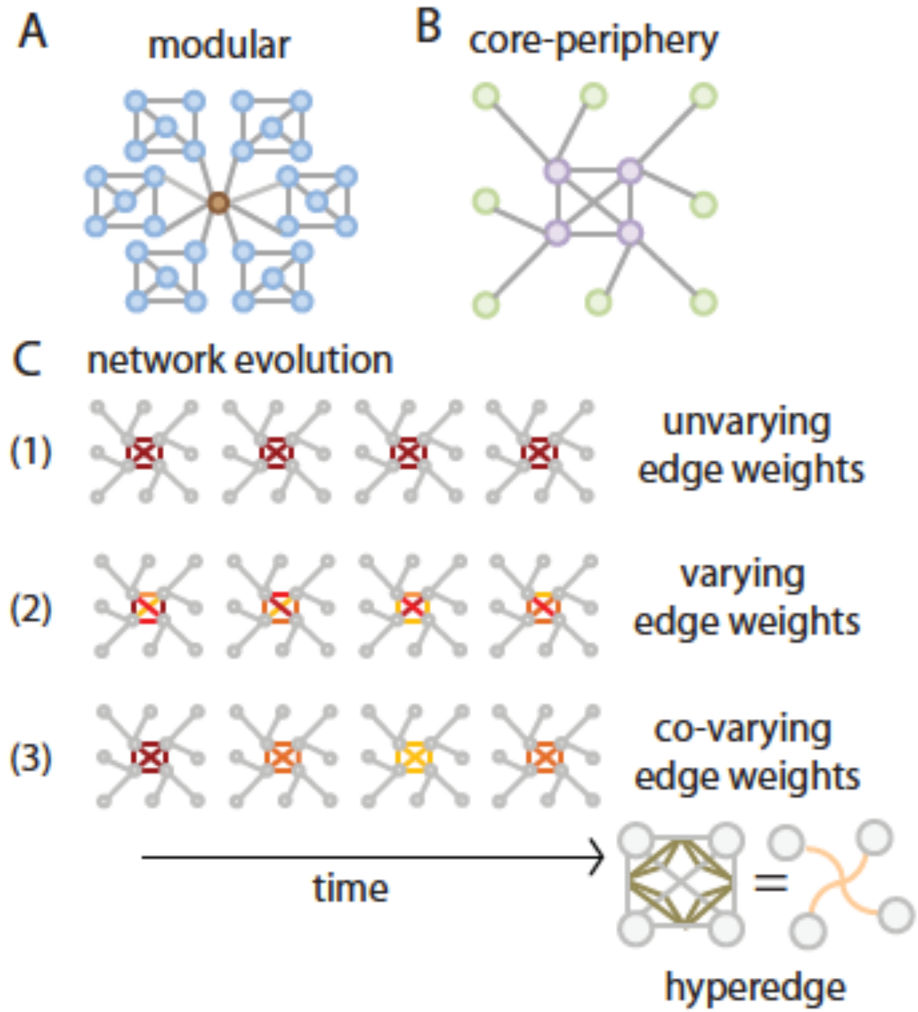
Temporal Core ≈ Structural Core!



Temporal core-periphery organization ≈ Structural core-periphery organization!

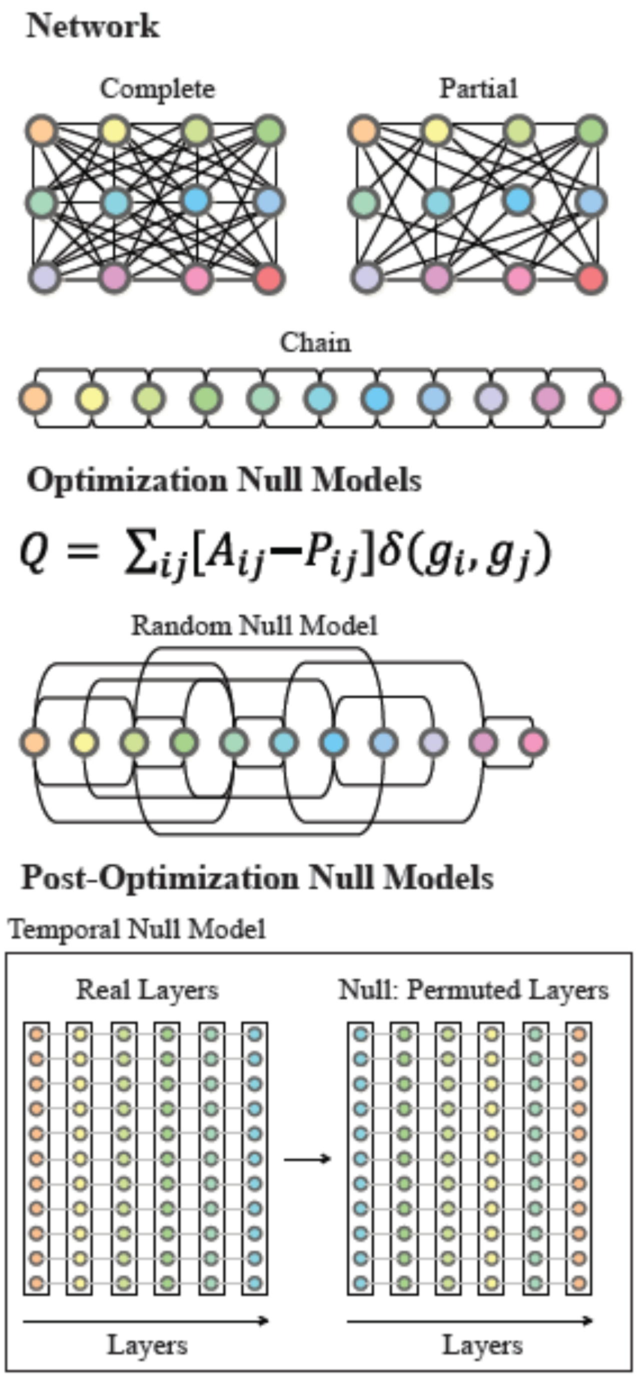
Cross-Links

- D. S. Bassett, N. F. Wymbs, MAP, P. J. Mucha, & S. T. Grafton, *Chaos*, **24**(1): 013112 (2014)
- Cross-links connect time-dependent edges to each other based on the similarity of their time series
  - Yield hyperedges that connect the associated nodes
- Try to discern which network evolution scenario occurs
  - Most hyperedges involve core (i.e. stiff) regions



Development of Null Models for Multilayer Networks

- D. S. Bassett, M. A. Porter, N. F. Wymbs, S. T. Grafton, J. M. Carlson, & P. J. Mucha, *Chaos*, **23**(1): 013142 (2013)
- Additional structure in adjacency tensors gives more freedom (and responsibility) for choosing null models.
- Null models that incorporate information about a system
  - E.g. chain null model fixes network topology but randomizes network “geometry” (edge weights)
- Also: Examine null models from shuffling time series directly (before turning into a network)
- Structural (γ) versus temporal resolution parameter (ω)
  - More generally, how to choose inter-layer (off-diagonal) terms C_{jrs}



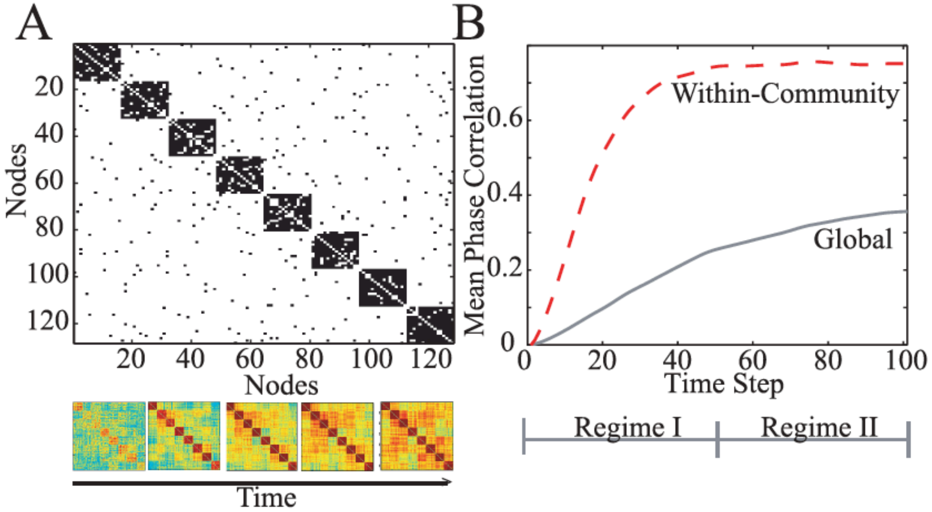
“The G. Bard Ermentrout Memorial Kuramoto Slide”

• Multislice community detection doesn’t care whether the time series come from experimental measurements or output from dynamical systems.

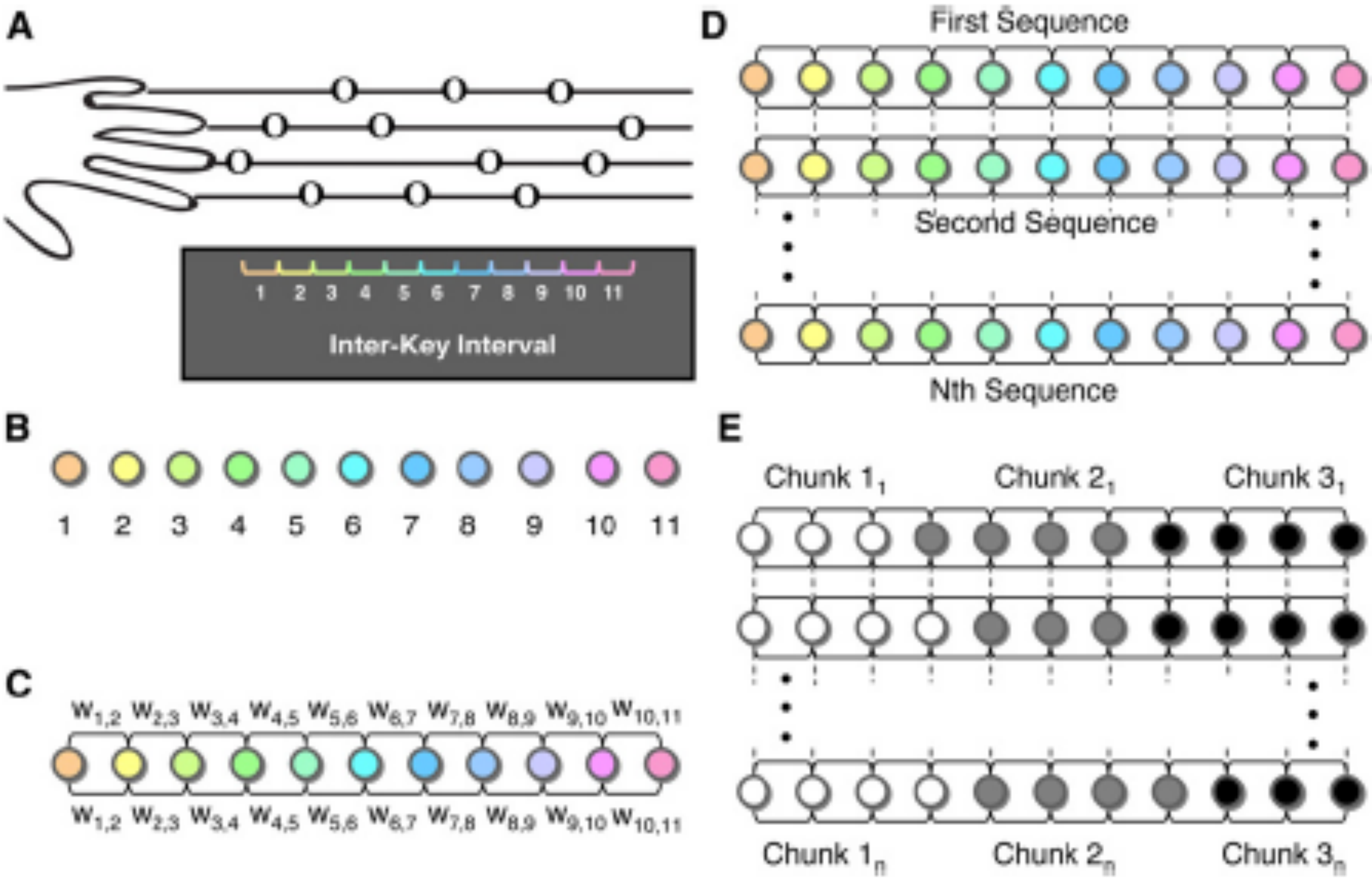
$$\frac{d\theta_i}{dt} = \omega_i + \sum_i \kappa A_{ij} \sin(\theta_j - \theta_i)\,, \quad i \in \{1, \ldots, N\}$$

$$\phi_{ij}(t) = \langle |\cos[\theta_i(t) - \theta_j(t)]| \rangle$$

• Leverage decades of knowledge on well-known dynamical systems to help with methodological development, validation, explore ideas, perhaps obtained insights on the dynamical systems themselves, etc.



Motor Chunking



N. F. Wymbs, D. S. Bassett, P. J. Mucha, M. A. Porter, & S. T. Grafton, *Neuron*, Vol. 74, No. 5, 936–946 (2012)

Conclusions

- Multilayer networks and tensors: their time has come
  - Our review article: M. Kivelä et al, *Journal of Complex Networks*, 2014
- Mesoscale structure of networks can be very insightful
  - E.g. community structure, core-periphery structure
- Generalization of community structure to time-dependent and multiplex networks allows investigation of more realistic situations while throwing away less data
- Insights on both brain and behavioral data
  - Dynamic reconfiguration of human brain networks during learning
    - Flexibility of nodes predicts simple motor learning
  - Good correspondence between structure and dynamics: flexible nodes in network periphery, and stiff nodes in network core
  - Discern time-evolving strategies for motor chunking
- Code available:
  - Code for Louvain optimization method for multislice modularity: http://netwiki.amath.unc.edu/GenLouvain
  - Code for visualizing networks: http://netwiki.amath.unc.edu/VisComms
  - Code for visualization and analysis of multilayer networks (various languages): http://www.plexmath.eu/?page_id=327
- Thanks: James S. McDonnell Foundation, EPSRC, FET-Proactive project "PLEXMATH"

Advertisements

Advertisement: 2015 "Sun"belt Conference (June 23–28, 2015, "Bright"on, UK)

- Matteo Magnani, Luca Rossi, and I have organized a special session on multilayer networks.
  - Please consider submitting a contributed talk.
- Conference website: http://insna.org/sunbelt2015/
- Description of our session: http://insna.org/sunbelt2015/?page_id=441
- (There's going to be a rumble in Brighton in June!)

Advertisement: Lake Como School on Complex Networks (May 17–21, 2015)

- Lake Como School of Advanced Studies:
  - http://lakecomoschool.org/
  - Applications due 3/15/15
- School on Complex Networks
  - The Boss: Carlo Piccardi
  - Scientific Board: Stefano Battiston, Vittoria Colizza, Peter Holme, Yamir Moreno, Mason Porter

Advertisement: Workshop on the Mathematics and Physics of Multilayer Complex Networks (MAPCOM15)

- Organizers: Alex Arenas, Mason Porter
- July 6–8, 2015, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany
- Applications due 3/31/15:
  - http://www.pks.mpg.de/~mapcom15/

Advertisement: MBI Semester Program on Networks (Spring 2016)

- Mathematical Biosciences Institute, The Ohio State University, USA
- Semester program on “Dynamics of Biologically Inspired Networks”
  - http://mbi.osu.edu/programs/emphasis-programs/future-programs/spring-2016-dynamics-biologically-inspired-networks/
- Focuses on theoretical questions on networks that arise from biology

Advertisement: MBI 2016, WP3

"Generalized Network Structures and Dynamics"

Organizers

Vittoria Colizza
Pierre Louis Institute of Epidemiology and Public Health, Universit'e de Paris VI (Pierre et Marie Curie)

Stephen Coombes
Department of Mathematics, University of Nottingham

Nina Fefferman
Department of Ecology, Evolution and Natural Resources, Rutgers University

Mason Porter
Mathematical Institute, University of Oxford

Description

The majority of current research efforts that explore network-based biological questions make a series of simplifying assumptions about the nature of the networks themselves. The primary purpose of such assumptions has been to enable the application of existing techniques from subjects such as graph theory and linear algebra rather than to enable either biological accuracy or rigorous examination of the mathematical impact of the simplifications. Within this class of assumptions, four assumptions have the greatest potential to compromise the generation of valid, novel biological understanding:

1. The network has only a single type of interaction among entities
2. The interactions among entities can be completely described as pairwise
3. The network is static over time
4. The impact of noise can be ignored

- March 21–25, 2016
- http://mbi.osu.edu/event/?id=898