Simultaneous prediction and community detection for networks with application to neuroimaging

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Joint work with Liza Levina

Outline

1. Introduction

2. Classification and prediction with network covariates

3. Simultaneous prediction and community detection with networks
   - Methodology
   - Algorithms for block-structured regularization
   - Theoretical properties
   - Simulations and brain network data

Outline

Networks

- **Graphs** are a popular structure to represent relational data
  - Vertices/nodes represent the units of a system.
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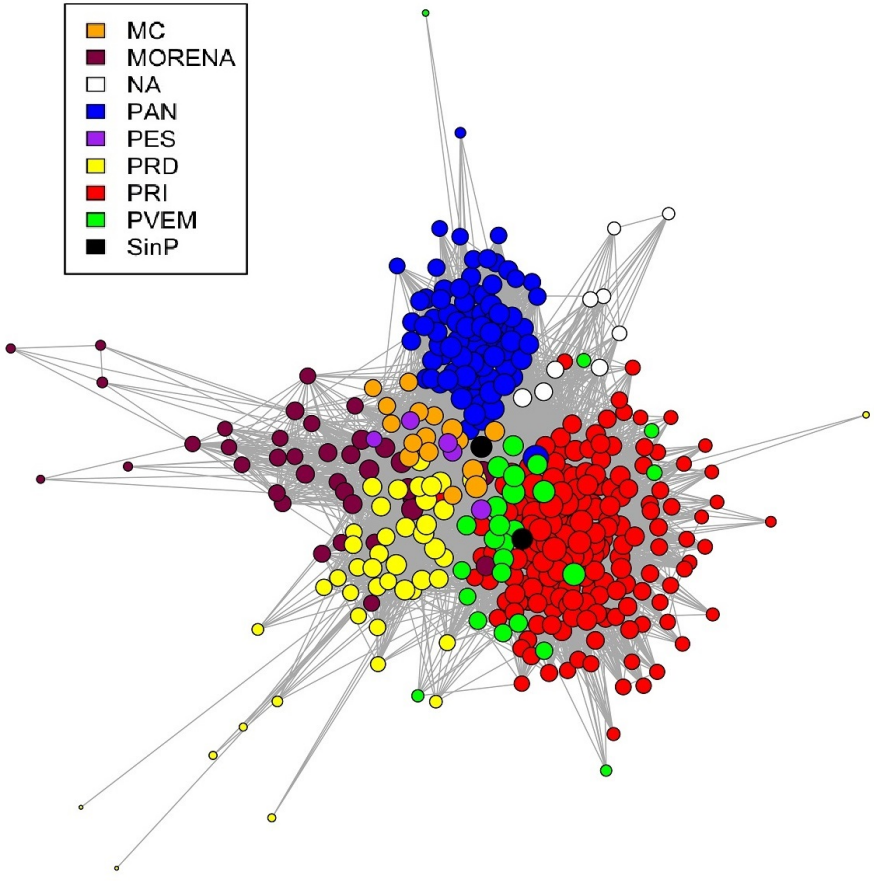
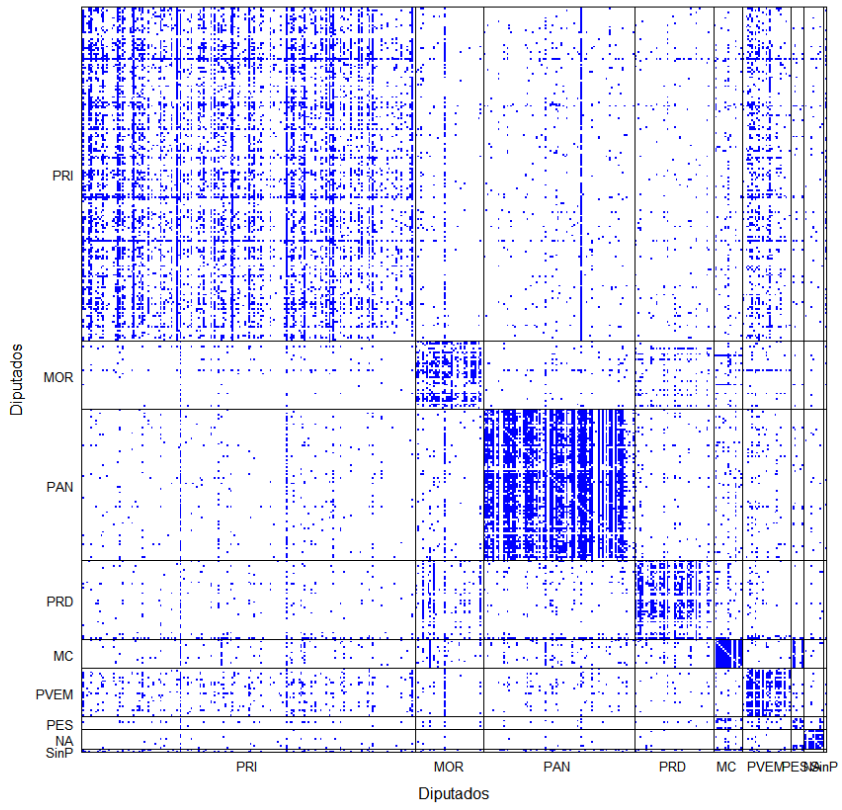
Mexican Representatives Twitter follow network (2018)

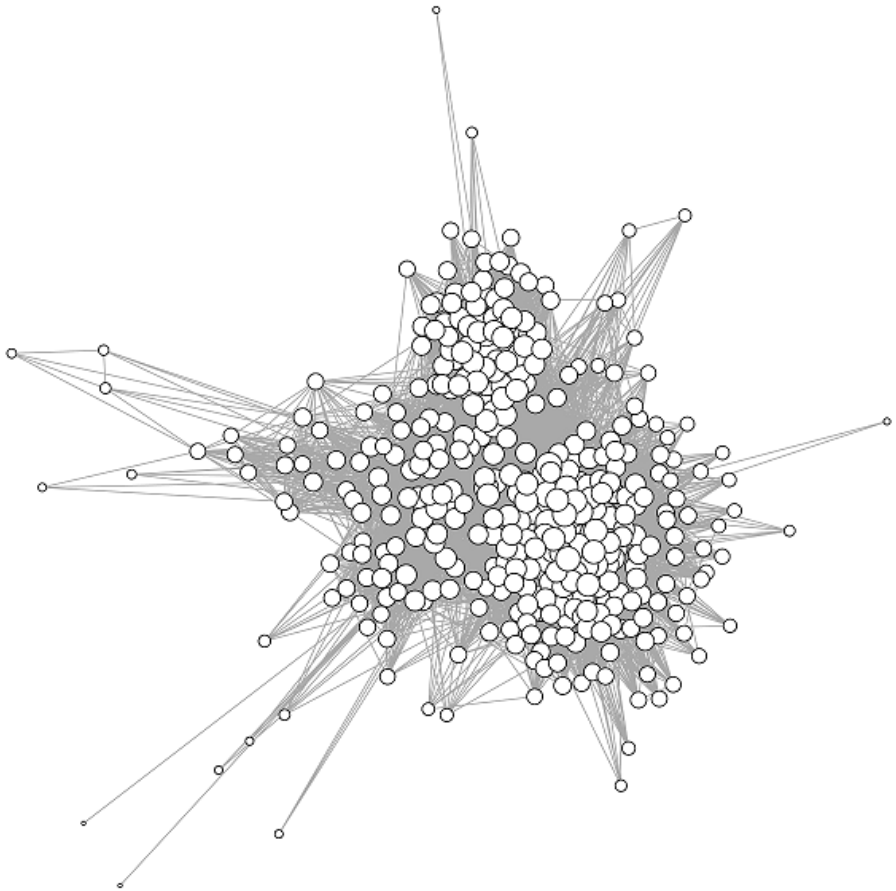




https://github.com/jesusdaniel/spcaCD/

Community detection

Goal: find meaningful groups of nodes (i.e. unsupervised clustering)



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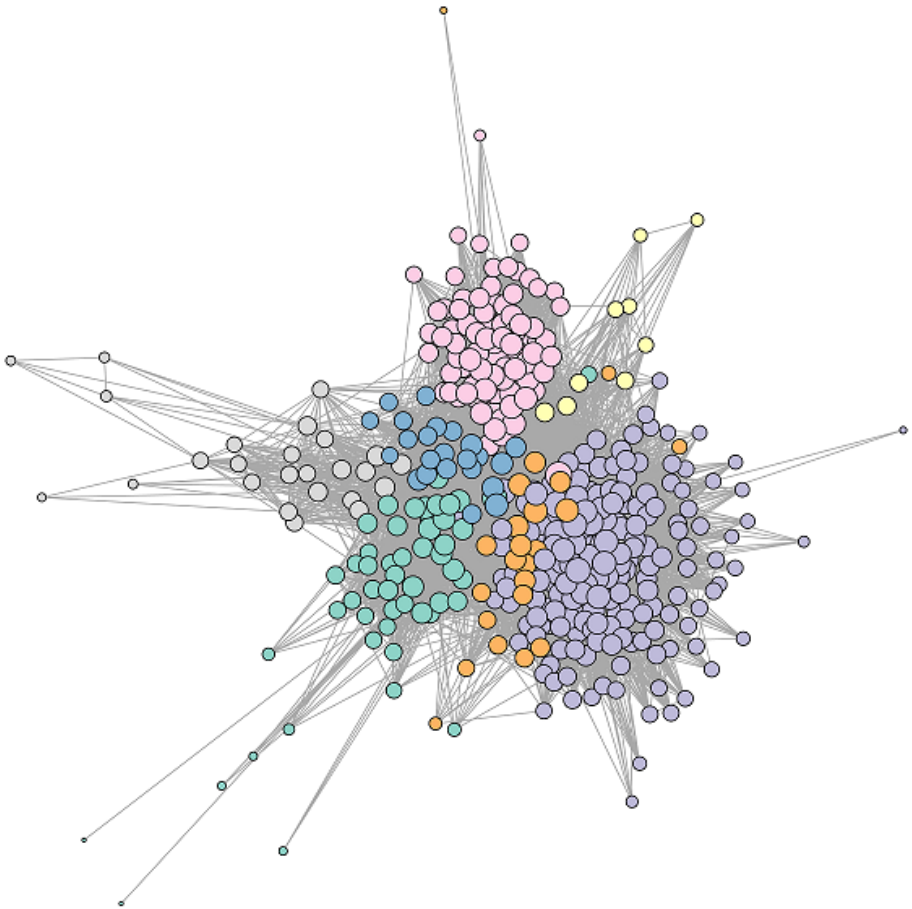

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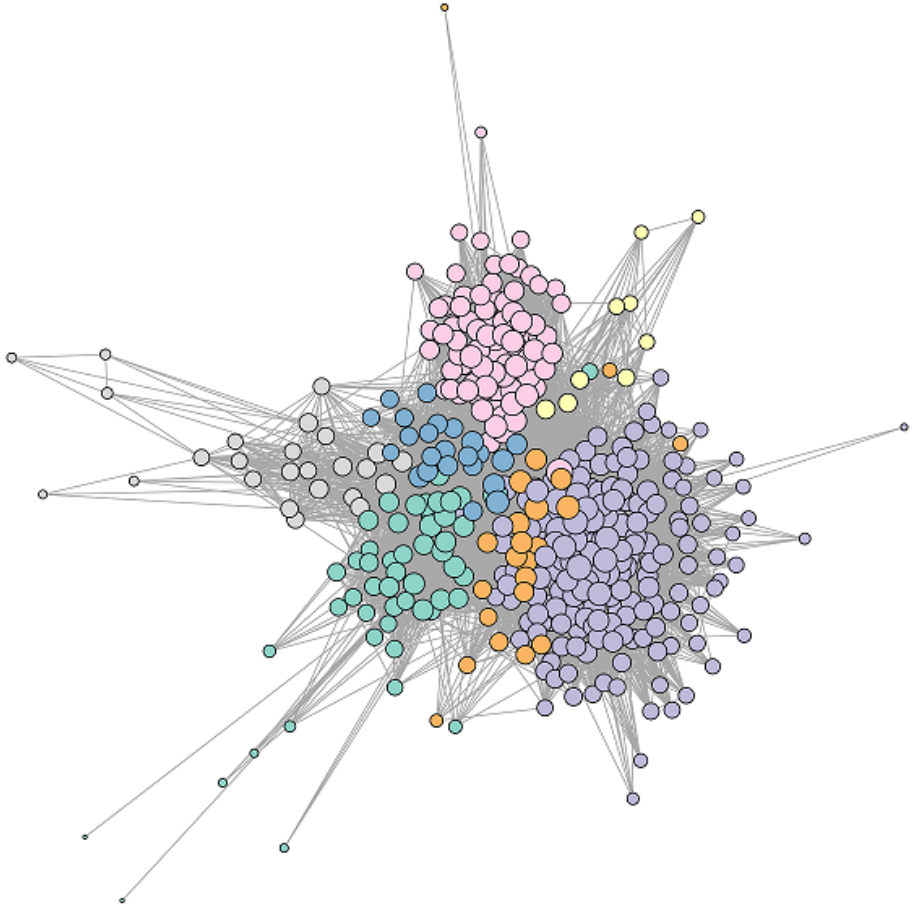

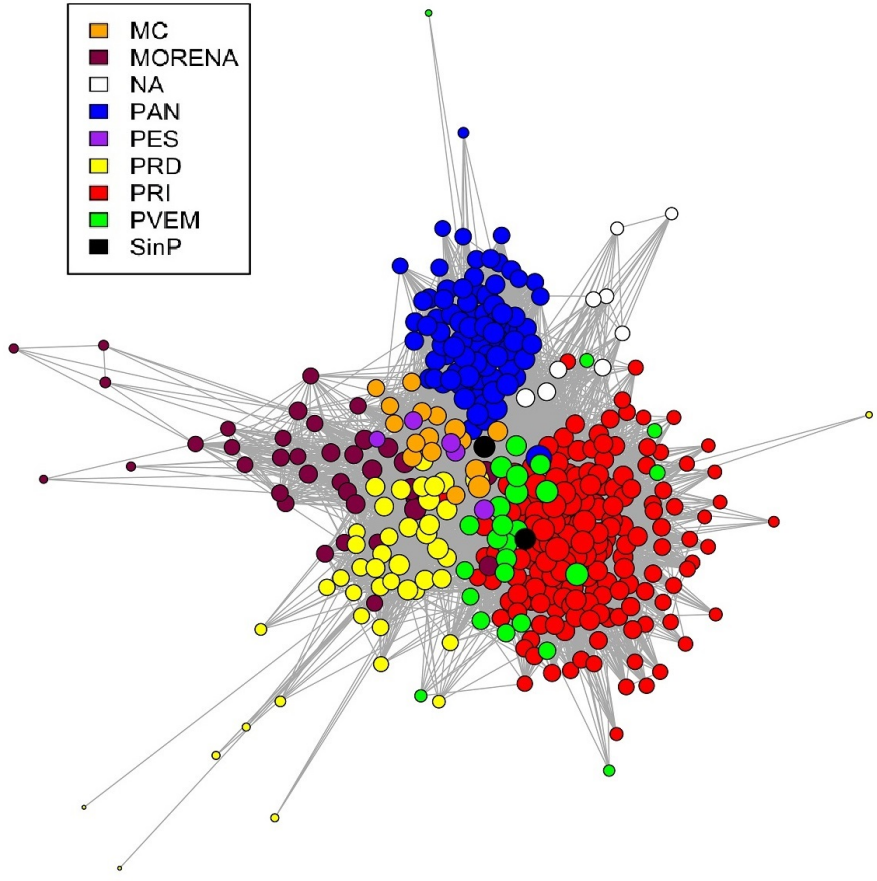

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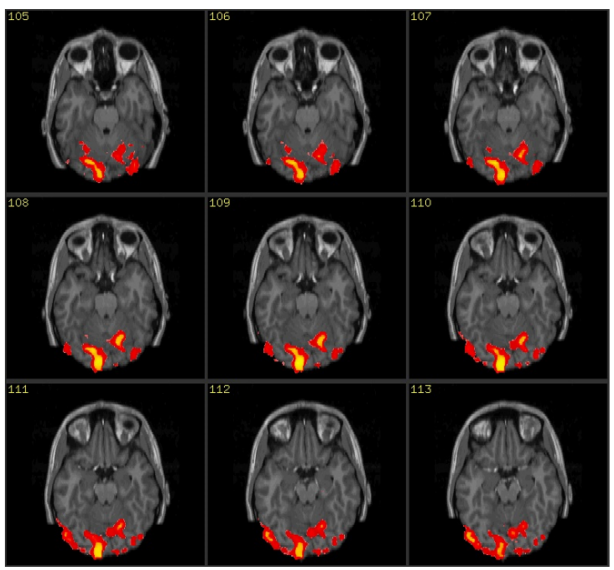
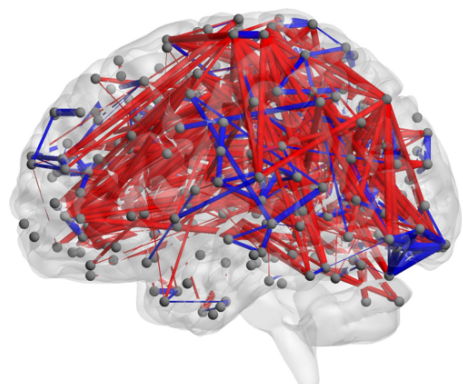
Brain networks

- Subject-specific networks constructed from imaging techniques
- Resting state fMRI data: time series of blood oxygenation level measurements
- Nodes: predefined locations in the brain (regions of interest, ROIs)
- Edges: a functional connectivity measure (Fisher-transformed marginal correlations)
- Pre-processing choices with big downstream effects: noise removal, registration, measures of connectivity





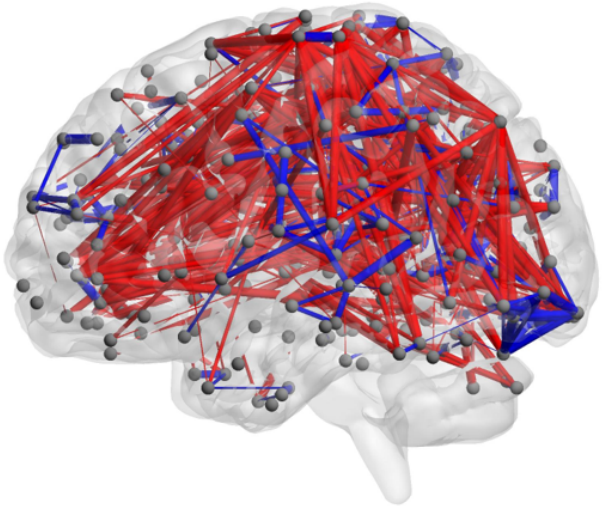
Community structure in the brain

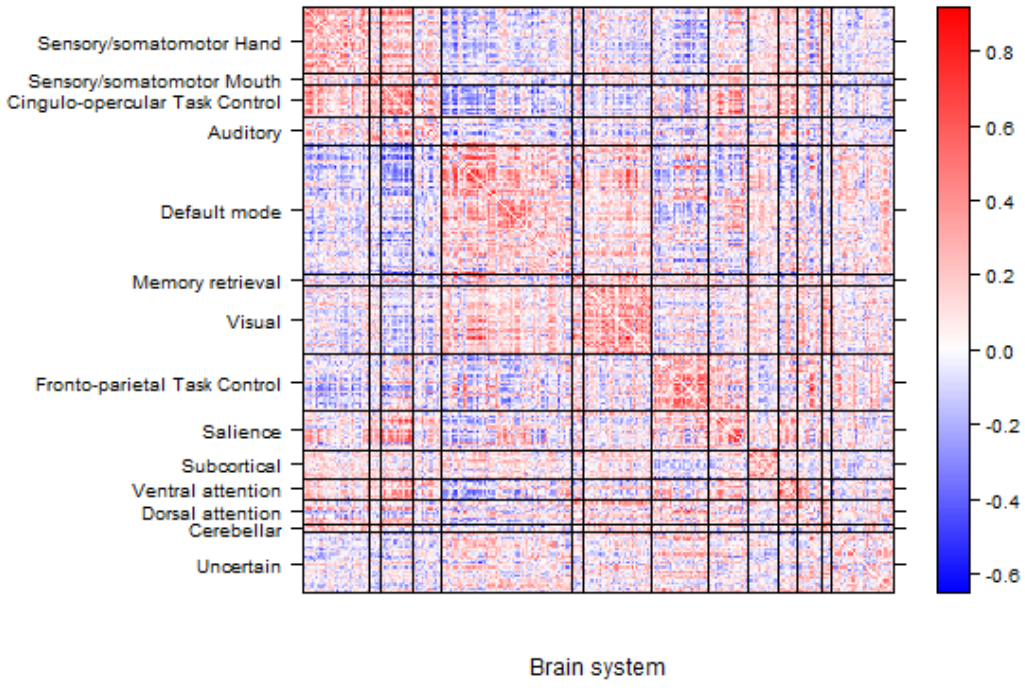
- Community detection algorithms are used to discover meaningful groups of nodes
- Communities correspond to functional brain systems: nodes activate together during tasks and have similar functionality

	Brain system	Nodes (total)
1	Sensory/somatomotor Hand	30
2	Sensory/somatomotor Mouth	5
3	Cingulo-opercular Task Control	14
4	Auditory	13
5	Default mode	58
6	Memory retrieval	5
7	Visual	31
8	Fronto-parietal Task Control	25
9	Salience	18
10	Subcortical	13
11	Ventral attention	9
12	Dorsal attention	11
13	Cerebellar	4
-1	Uncertain	28

Correspondence between communities and functional systems (Power et al., 2011)

Community structure in the brain





Brain network from a subject in the COBRE dataset (Aine et al., 2017)

Community detection: a short summary

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  - Likelihood-based approaches
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  - Maximization of an objective function (modularity, random-walk objectives)
- In practice, different algorithms might yield different but meaningful communities (Priebe et al., 2019)
- How can we identify meaningful communities for the problem of interest?

Multiple network data

- In many applications, a collection of graphs with matched vertices is observed:
  - Multilayer networks
  - Time-varying networks
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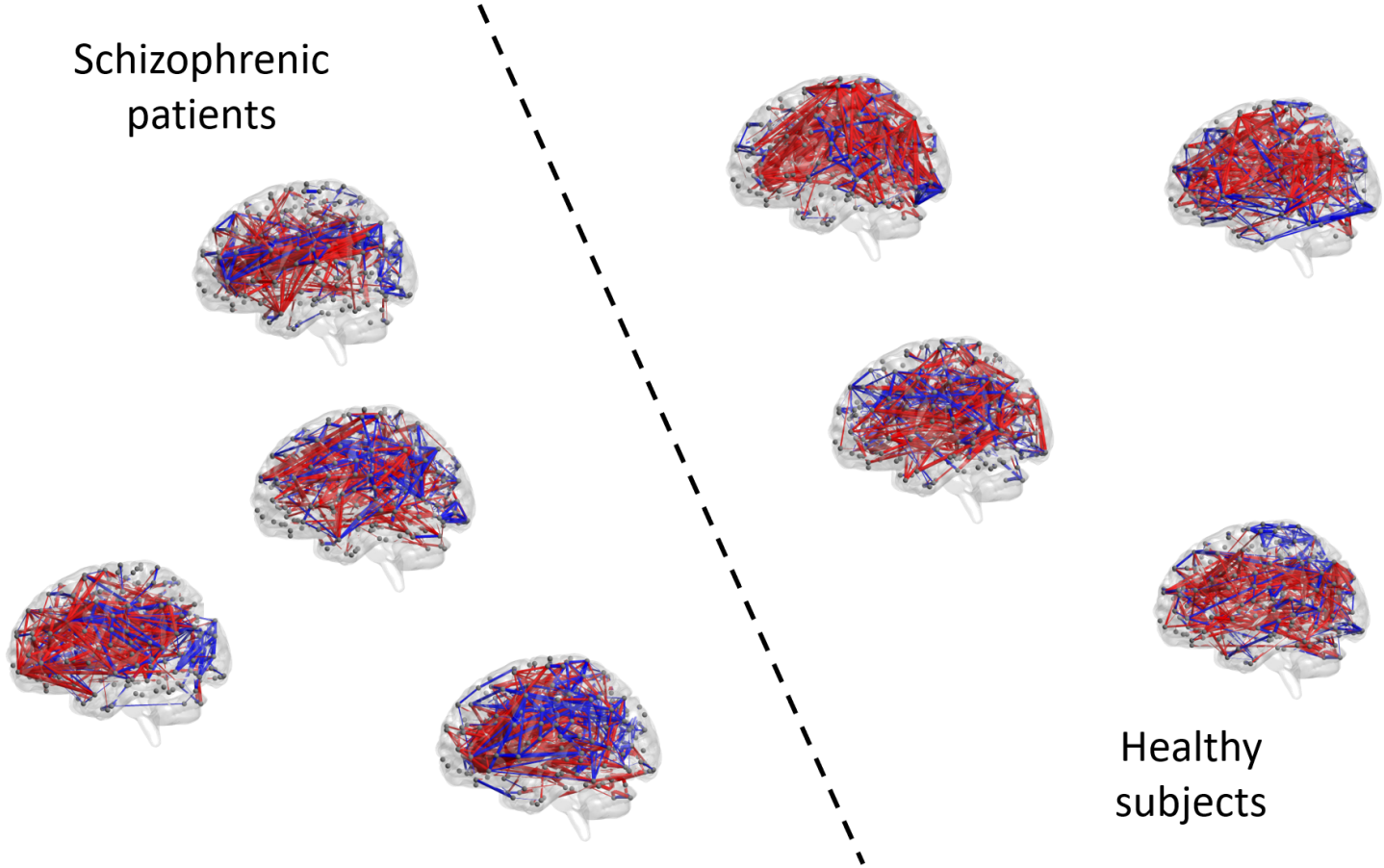
- How do we incorporate the network structure of the data?
- Often, there are network-specific attributes, and there is interest in understanding the relationship between the connectivity and these attributes

Classification of brain networks



Outline

Setting and notation

Setting: sample of graphs with matched vertices

- n nodes
- m graphs
- $A^{(1)}, \ldots, A^{(m)}$ adjacency matrices (size $n \times n$)
  - Weighted entries ($\mathbb{R}^{n \times n}$)
  - Symmetric
  - Zero-diagonal
- Additional network-specific labels or responses $Y_1, \ldots, Y_m$
  - $Y_i \in \{0, 1\}$ or $Y_i \in \mathbb{R}$

Problem:

- Predict a response Y using the network information A
- Understand the relationship between A and Y

Prediction with network covariates

Two popular approaches to analyzing multiple networks (Bullmore and Sporns, 2009):

1. **Global network summaries** used as features
   - Degree, clustering coefficient, average path length, etc.
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   - Standard statistical tools can be applied
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Our goal: develop statistical tools for jointly analyzing samples of networks

- Use local information but incorporate network structure.
- Parsimonious and interpretable solutions.
- Efficient computation and theoretical guarantees.

Methodology

- Linear prediction model for the response (e.g. GLM):

$$\mathbb{E}[Y_i|A^{(i)}] = f(\langle A^{(i)}, B\rangle) = f(\mathsf{Tr}(B^T A^{(i)}))$$

  - Connectivity matrix $\rightarrow$ a linear combination of edge weights
  - $B \in \mathbb{R}^{n\times n}$ symmetric matrix of coefficients.
  - f link function

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- In general, B is estimated by minimizing some loss function

$$\ell(B) = \frac{1}{m}\sum_{i=1}^{m} \ell(Y_i, \langle A^{(i)}, B\rangle)$$

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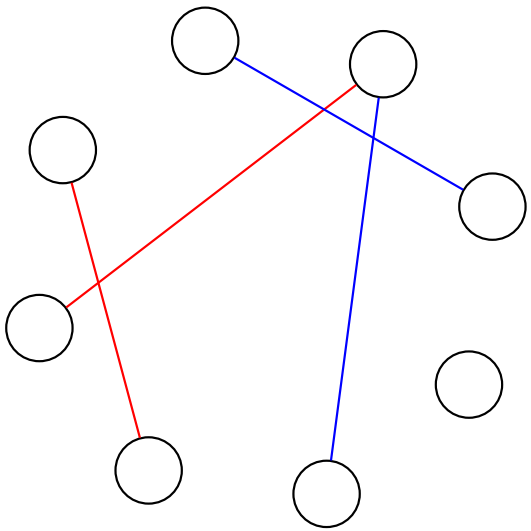
- High-dimensional problem: usually $m \ll n^2$.
- Enforce structure and sparsity in the solution through constraints and penalties

$$\hat{B} = \underset{B\in\mathcal{B}}{\operatorname{argmin}} \{\ell(B) + \Omega_\lambda(B)\}$$

Parsimony in network coefficients (initial approach)



Edge sparsity: small subset of predictive edges

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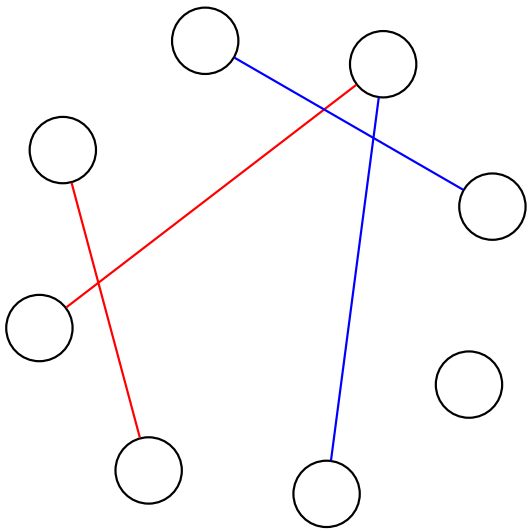
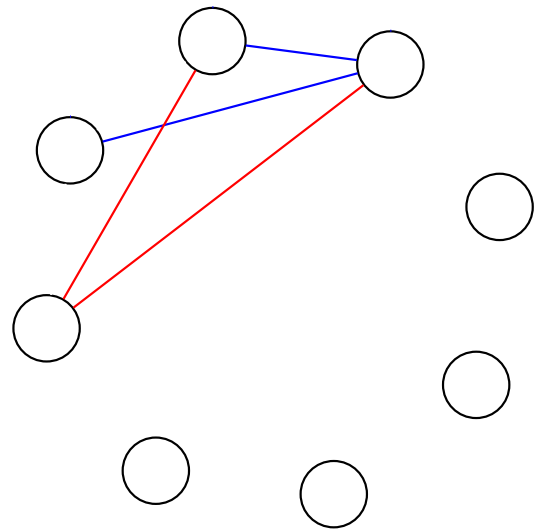
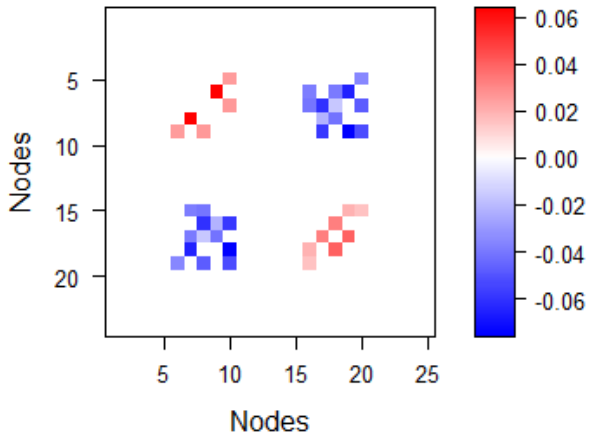


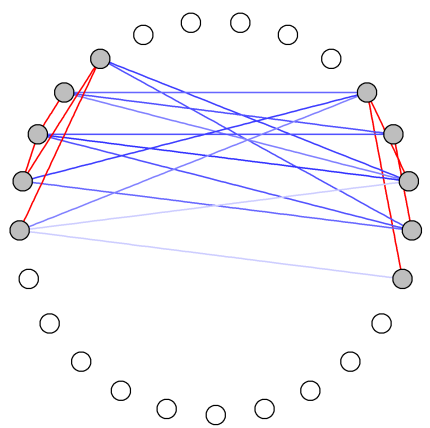
Edge sparsity: small subset of predictive edges



Node sparsity: small subset of nodes with predictive edges

Edge and node selection with overlapping group lasso (Arroyo Relión et al., 2019)

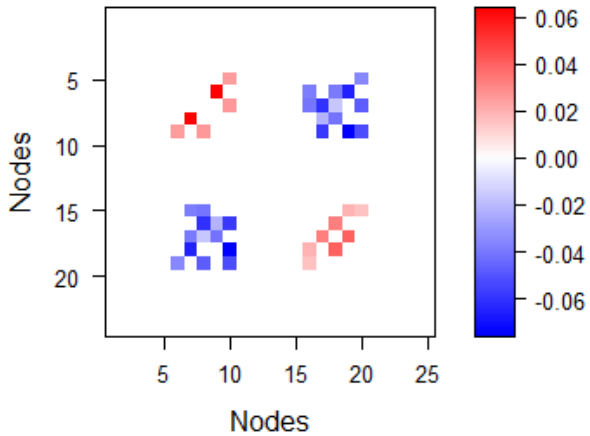




- **Edge selection:** lasso penalty
- Active node: at least one of its edges selected
- **Node selection:** penalize active nodes using group lasso.

$$\Omega_{\lambda,\rho}(B) = \lambda \left(\sum_{i=1}^{n} \sqrt{B_{i1}^2 + \ldots + B_{in}^2} + \rho \sum_{i,j} |B_{ij}| \right).$$

Edge and node selection with overlapping group lasso (Arroyo Relión et al., 2019)



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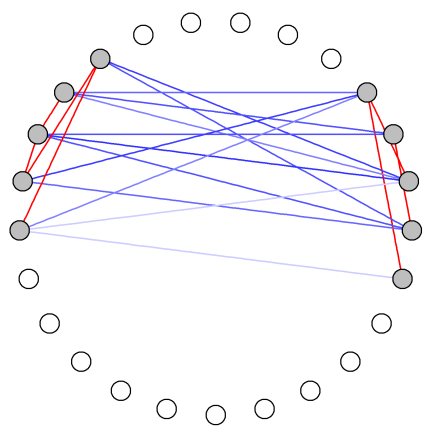


Proposition

Under regularity conditions, we have

- Consistency: $\|\widehat{B} - B^*\|_F^2 = O_P\left(\frac{G^2 \log N}{n}\right)$
- Node false discovery control: $\hat{\mathcal{G}} \subset \mathcal{G}$ w.h.p.

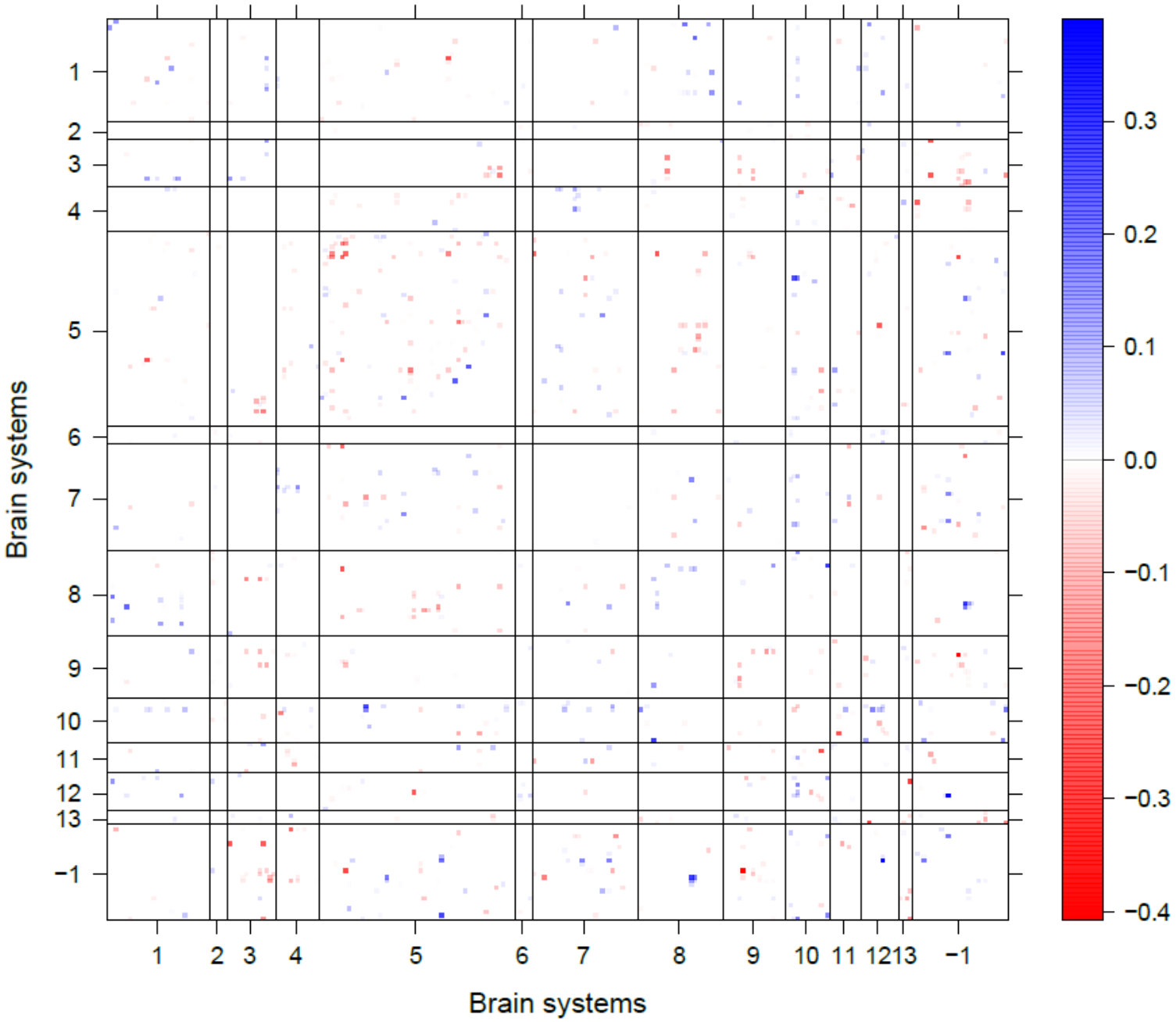
Schizophrenia classification

- COBRE dataset (Aine et al., 2017)
  - 54 schizophrenia patients, 70 healthy subjects ($m = 124$)
  - $m = 263$ regions of interest (nodes) and 34,453 edges
- Good accuracy with a substantially reduced set of edges ($\sim 1,000$).

Method	**% Acc. (s.e.)**
With variable selection	
Our method	92.7 (2.6)
Elastic net	89.5 (1.8)
SVM-L1	87.9 (2.2)
Signal-subgraph	86.1 (3.3)
DLDA	84.6 (3.3)
Lasso	80.1 (5.6)
No variable selection	
SVM	93.5 (2.1)
Ridge penalty	91 (2.6)
Random forest	74.2 (2.6)
Network summaries	64.5 (3.8)

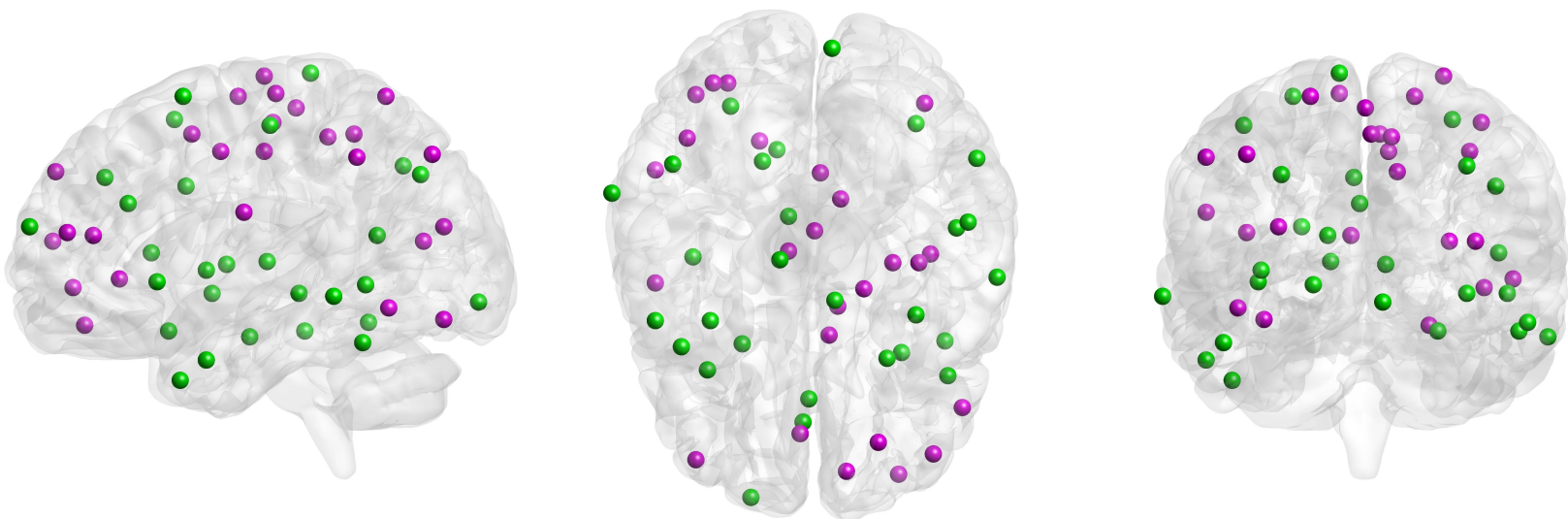
10-fold cross-validation accuracy (standard error)

Matrix of fitted coefficients



Variable selection

- Stability selection (Meinshausen and Buhlman, 2010) to investigate variable selection probabilities.
- Many of the most selected nodes (green) appear in the default-mode network (5) and fronto-parietal task control region (8).
- At least 25 nodes that are consistently not selected for prediction (purple).



Prediction with node selection

- Network-informed penalties improve accuracy and variable selection
- High correlations among edge-variables within a community
- Results are typically interpreted at the community level
- Can we incorporate the community structure in the regularization?

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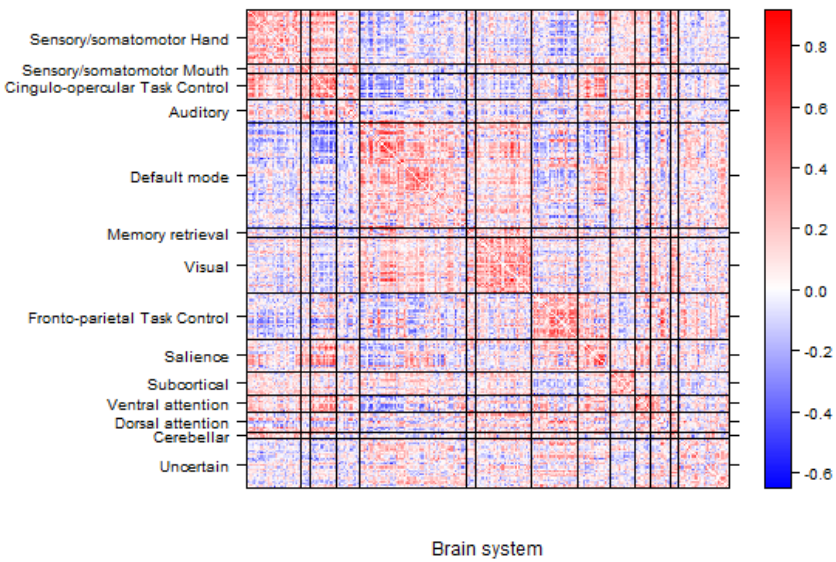
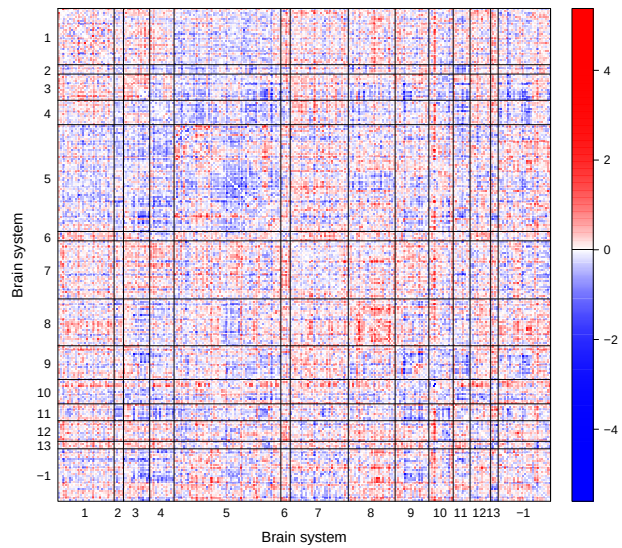
Community structure in brain networks

- Brain systems are usually derived from healthy subjects.
- They may not fully capture differences between conditions.



A brain network
from a healthy subject



t-statistics for schizophrenic
vs. healthy subjects

Supervised community detection

- Neuroscientific evidence of association between subject-level phenotypes (age, gender, mental illnes) and brain organization (Meunier et al., 2009, Sripada et al. 2014, Kessler et al. 2016)
- Reconfiguration of the brain according to task-induced states (Salehi et al., 2019)
- More generally, clustering is ill-defined, and is usually guided by the problem of interest

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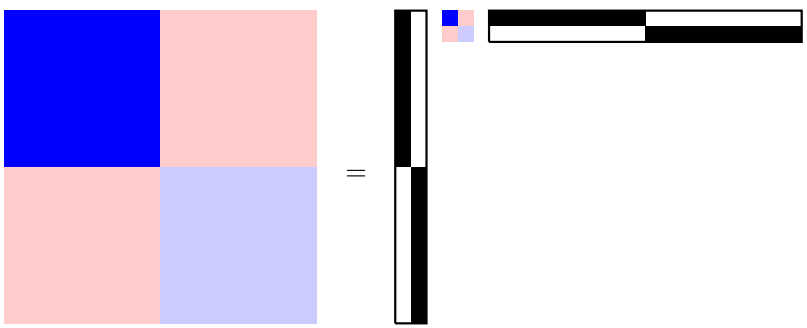
Our goals:

- Learn community structure and prediction rule simultaneously
- Find network cells with the best predictive power for a specific response of interest

Block structure in coefficients

- Enforce community structure in the coefficients B:
  - Partition the nodes into K groups (communities)
  - Constraint $B = ZCZ^\top$ b



- Community membership matrix: $Z \in \{0,1\}^{n \times K}$, $\sum_{k=1}^{K} Z_{jk} = 1$
- Coefficients: $C \in \mathbb{R}^{K \times K}$
- Analogous to the stochastic block model (SBM)

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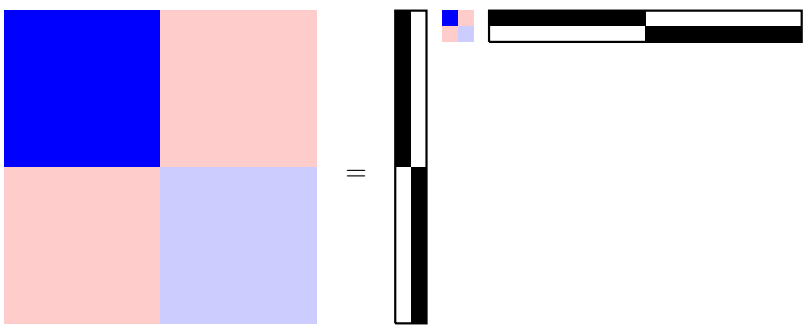

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- Coefficients are clustered into cells with similar predictive behavior.
- Communities simplify interpretation (from $O(n^2)$ to $O(K^2)$ coefficients)

Optimization problem

- Given a value of $K < N$, optimize

$$\begin{aligned} \min_{Z,C} \quad & \ell(ZCZ^\top) + \Omega_\lambda(ZCZ^\top) \\ \text{subject to} \quad & Z \in \{0,1\}^{n \times K}, \qquad Z\mathbf{1}_K = \mathbf{1}_N \\ & C \in \mathbb{R}^{K \times K} \end{aligned}$$

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Strategy:

1. Spectral clustering: provides a good initialization value
2. Apply an iterative optimization algorithm (ADMM)

Spectral clustering

- Assume that edge weights are centered and standardized across the sample

$$\sum_{i=1}^{m} A_{uv}^{(i)} = 0, \qquad \frac{1}{m}\sum_{i=1}^{m} (A_{uv}^{(i)})^2 = 1.$$

- We focus on the least-squares loss function

$$\ell(B) = \frac{1}{2m}\sum_{i=1}^{m} \Big(Y_i - \mathsf{Tr}(B^T A^{(i)})\Big)^2$$

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- We focus on the least-squares loss function

$$\ell(B) = \frac{1}{2m}\sum_{i=1}^{m}\left(Y_i - \mathsf{Tr}(B^T A^{(i)})\right)^2$$

- Define $\widehat{\Sigma}^{\mathcal{A},\mathcal{Y}} \in \mathbb{R}^{n\times n}$ as the OLS estimate for uncorrelated predictors

$$(\widehat{\Sigma}^{\mathcal{A},\mathcal{Y}})_{u,v} = \widehat{\mathsf{Cov}}(A_{uv}, Y) = \frac{1}{m}\sum_{i=1}^{m} Y_i A_{uv}^{(i)}.$$

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- This methods ignores the correlations between edges in the hope that highly correlated edges have similar weights on $\widehat{\Sigma}^{\mathcal{A},\mathcal{Y}}$

When does spectral clustering work?

Assumption 1 Centered and standardized covariates

$$\mathbb{E}\left[\sum_{i=1}^{m} A_{uv}^{(i)}\right] = 0, \qquad \mathbb{E}\left[\frac{1}{m}\sum_{i=1}^{m}(A_{uv}^{(i)})^2\right] = 1$$

Assumption 2 Linear model with block-constant coefficients and sub-Gaussian noise

$$Y_i = \mathsf{Tr}(B^T A^{(i)}) + \sigma\epsilon_i,$$

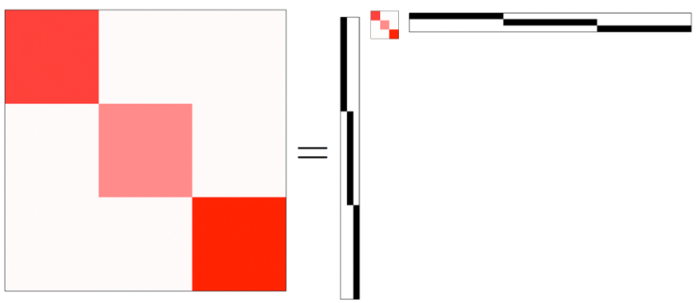
where $B = ZCZ^\top$.

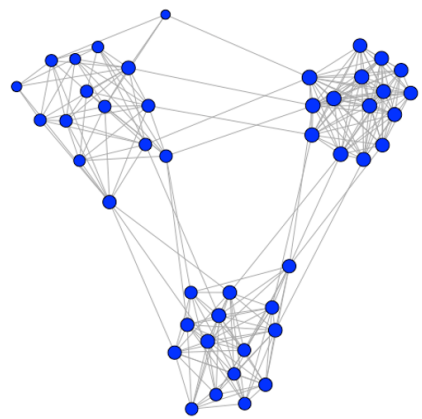
When does spectral clustering work?

Assumption 3 Weighted sub-Gaussian stochastic block model:

- Common membership matrix $Z \in \{0,1\}^{n \times K}$
- Symmetric $K \times K$ matrices $R^{(1)}, \ldots, R^{(m)}$ and $\Psi^{(1)}, \ldots, \Psi^{(m)}$
- $\{A_{uv}^{(m)}\}$ are independent sub-Gaussian r.v. and

$$\mathbb{E}[A^{(i)}] = ZR^{(i)}Z^\top, \qquad \mathsf{Var}(A_{uv}^{(i)}) = (Z\Psi^{(i)}Z^\top)$$





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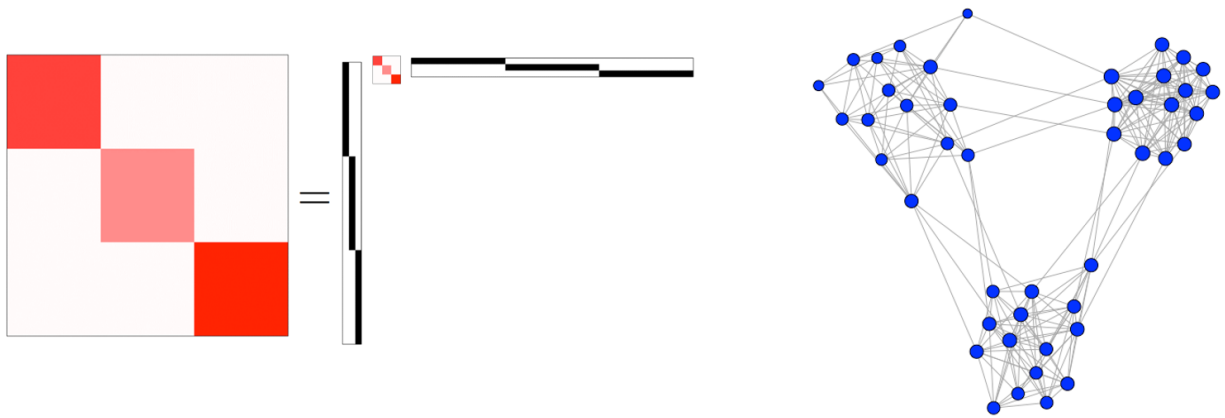

- $\Sigma^{\mathcal{A}}_{[u,v],[s,t]} = \mathbb{E}\left[\frac{1}{m}\sum_{i=1}^m A_{uv}^{(i)} A_{st}^{(i)}\right]$ is the covariance between edge variables
- Under this model, the covariance between edges only depends on community memberships

$$\Sigma^{\mathcal{A}}_{[u,v],[s,t]} = \frac{1}{m}\sum_{i=1}^m R^{(i)}_{z(u),z(v)} R^{(i)}_{z(s),z(t)}.$$

Consistency of spectral clustering

Theorem

Under regularity conditions, when $n_{min} \asymp n_{max}$*, the estimated membership matrix by spectral clustering satisfies*

$$\mathbb{E}\left[\|\widehat{\mathbf{Z}} - \mathbf{Z}\|_F\right] \lesssim \frac{K^{1/2} n^{3/2} \|B^*\|_F}{m^{1/2} \lambda_K(\mathbb{E}[\widehat{\Sigma}^{\mathcal{A},\mathcal{Y}}])} \left(1 + \frac{\sigma}{n\|B^*\|_F}\right)$$

as n *goes to infinity.*

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as n goes to infinity.

- When the correlation between edges on different cells ($\Sigma^{\mathcal{A}}_{[u,v],[s,t]}$) is bounded from above, then $\lambda_K(\mathbb{E}[\widehat{\Sigma}^{\mathcal{A},\mathcal{Y}}]) \asymp (n/K)^2 \lambda_{\min}(C^*)$.
- If $\lambda_{\min}(C)$ is bounded away from zero, then

$$\mathbb{E}\left[\|\widehat{\mathbf{Z}} - \mathbf{Z}\|_F\right] \lesssim \frac{K^{5/2} \|B^*\|_F}{m^{1/2} n^{1/2}} \left(1 + \frac{\sigma}{n\|B^*\|_F}\right)$$

Optimization via ADMM

- Introduce new variables and a parameter $\rho > 0$
  - $V \in \mathbb{R}^{n \times n}$
  - $W \in \mathcal{W} = \{ZCZ^T : Z \text{ is a membership matrix}, C \in \mathbb{R}^{K \times K}\}$

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- Iterate until convergence

$$B^{(t+1)} = \underset{B}{\operatorname{argmin}} \left\{ \ell(B) + \Omega_\lambda(B) + \frac{\rho}{2} \|B - (W^{(t)} - \frac{1}{\rho} V^{(t)})\|_F^2 \right\} \tag{1}$$

$$W^{(t+1)} = \underset{W \in \mathcal{W}}{\operatorname{argmin}} \left\| W - (B^{(t+1)} + \frac{1}{\rho} V^{(t)}) \right\|_F^2 \tag{2}$$

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- Problem is non-convex, use spectral clustering for a good initial value.
- Efficient updates
  - $B^{(t+1)}$ is the solution of a convex problem.
  - Solving for $W^{(t+1)}$ requires combinatorial optimization
    - ⋆ We approximate the solution via spectral clustering

Simulations

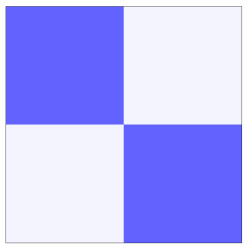
- Parameters that affect complexity of the problem
  - Regression noise
  - Correlation between edge variables
  - Sample size

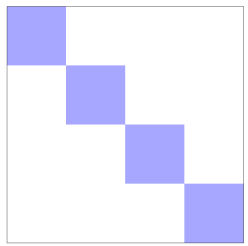
Simulations

- Parameters that affect complexity of the problem
  - Regression noise
  - Correlation between edge variables
  - Sample size
- Generate m weighted networks with $n = 40$ nodes and 4 communities

$$U_i \sim \text{Uniform}(-0.5, 0.5)$$

$$\mathbb{E}[A^{(i)}|U_i] = \quad + tU_i$$

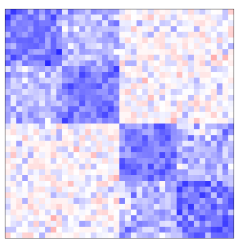


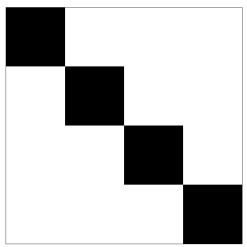


$$A_i = \mathbb{E}[A^{(i)}|U_i] + 0.1 \times Z, \quad Z \sim N(0, 1)$$

- Generate response using the linear regression model

$$Y_i = \left\langle \quad , \quad \right\rangle + \sigma\epsilon_i, \qquad \epsilon_i \sim N(0, 1).$$





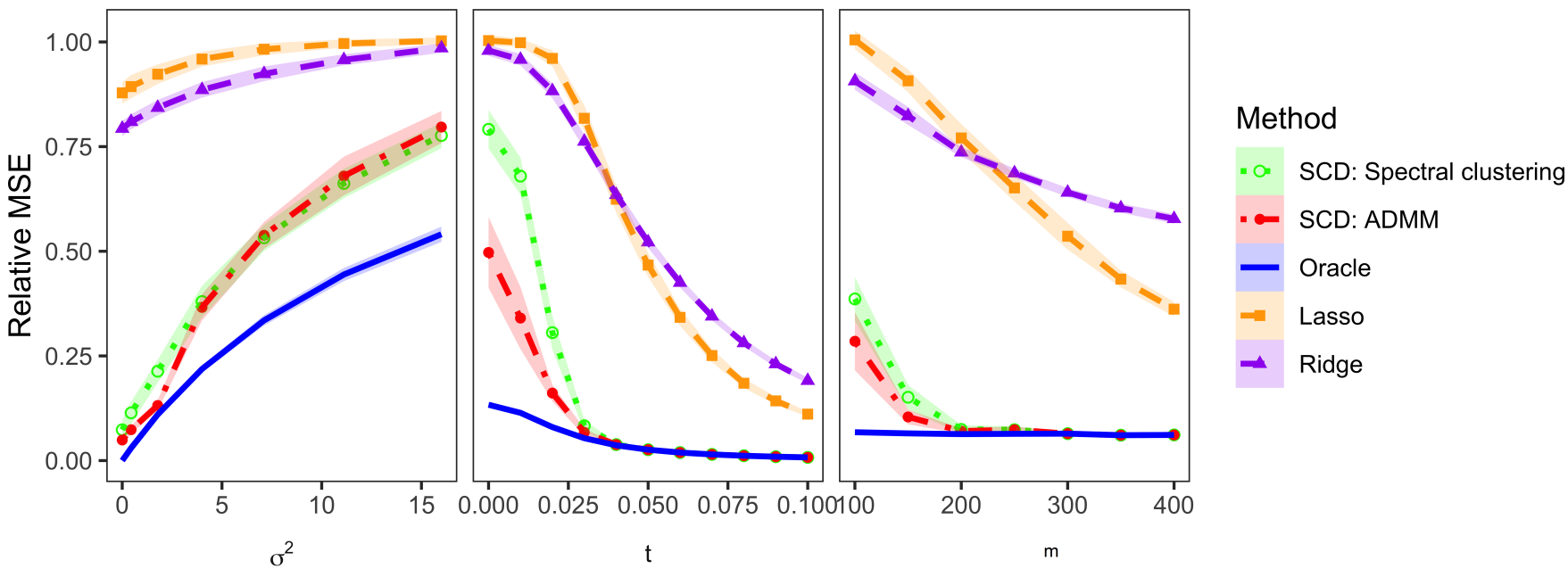
- Set $(\sigma^*, t^*, m^*) = (1, 0.025, 150)$ (low signal) and vary one parameter at a time

Simulations: prediction

- Prediction accuracy measured by relative MSE on a held-out set

$$\text{RMSE} = \frac{\sum_{i=1}^{m}(Y_i - \hat{Y}_i)^2}{\hat{\sigma}^2}$$

- Prediction benchmarks:
  - Lasso and ridge regression (no network structure)
  - An oracle that knows true communities

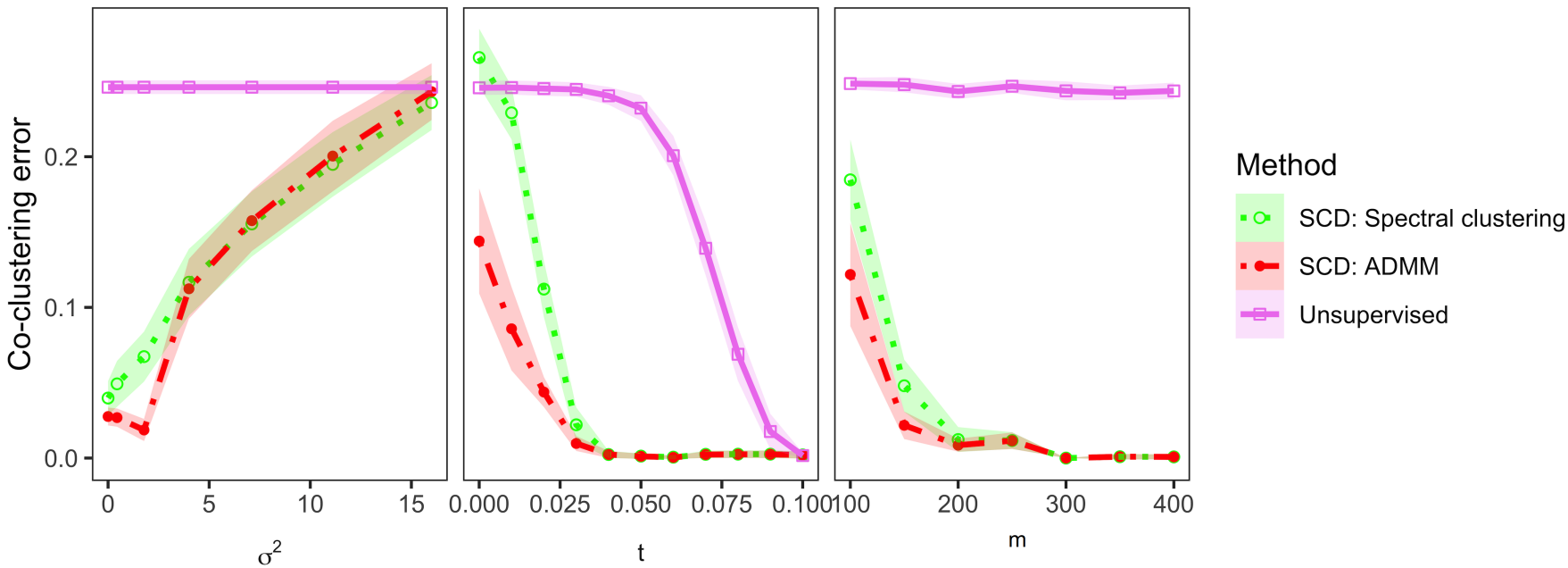


Simulations: community detection

- Community detection accuracy measured by co-clustering error

$$E(Z, \hat{Z}) = \frac{1}{m^2} \sum_{i=1}^{m} \sum_{j=1}^{m} (ZZ^T - \hat{Z}\hat{Z}^T)_{ij}$$

- Community detection benchmark (unsupervised)
  - Spectral clustering for multiple sparse networks (Bhattacharyya and Chatterjee, 2018): spectral clustering on the sum of squared adjacency matrices



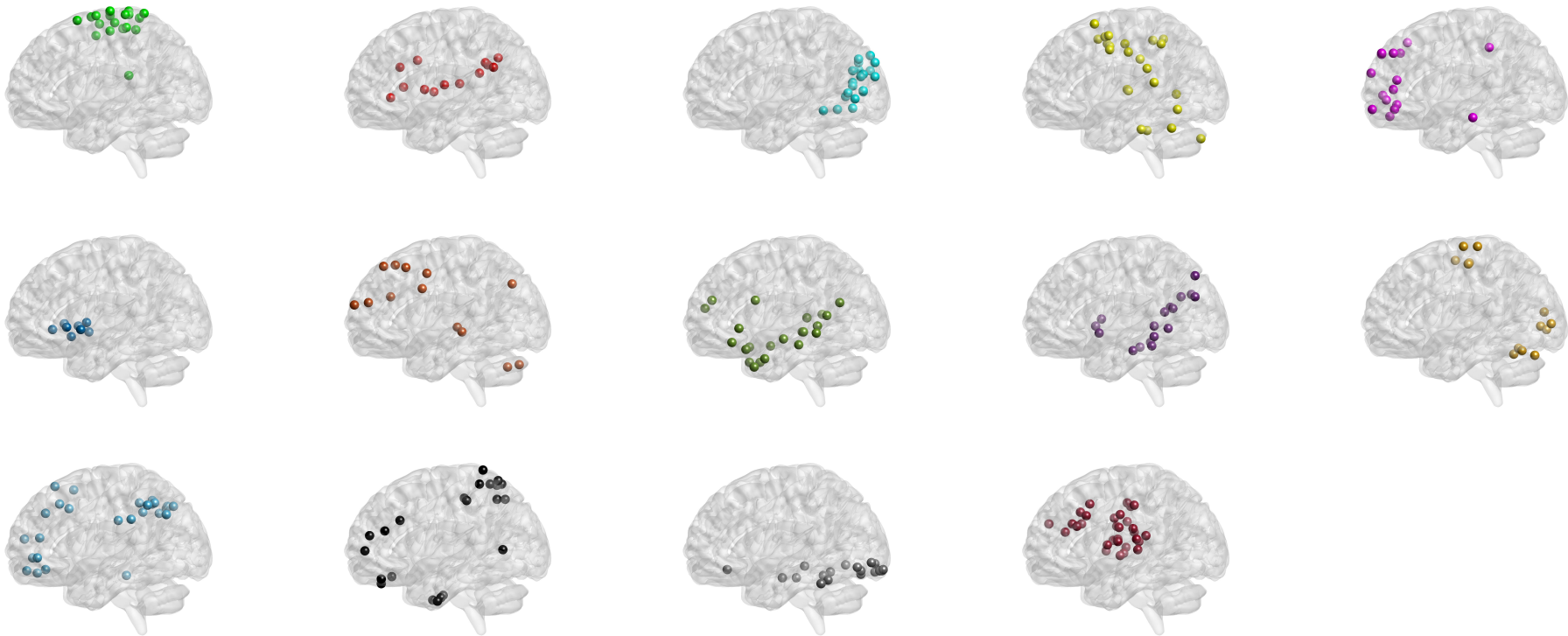
Schizophrenia classification

- Supervised community detection with logistic loss and a lasso penalty
- Accuracy evaluated on COBRE dataset
- Benchmark: Power et al. (2011) communities (14 brain systems)
- Supervised community detection using $K = 14$ communities shows superior performance in accuracy with the same number of parameters.

Power brain systems
CV accuracy: 62%

Supervised community detection
CV accuracy: 79%

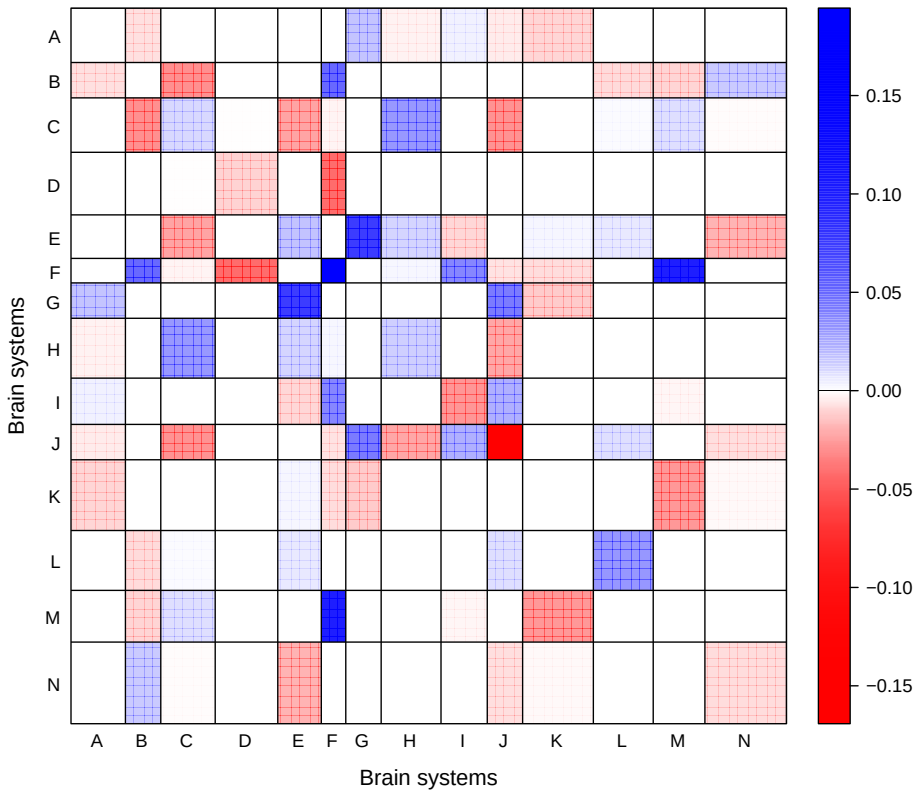
Supervised communities in COBRE data



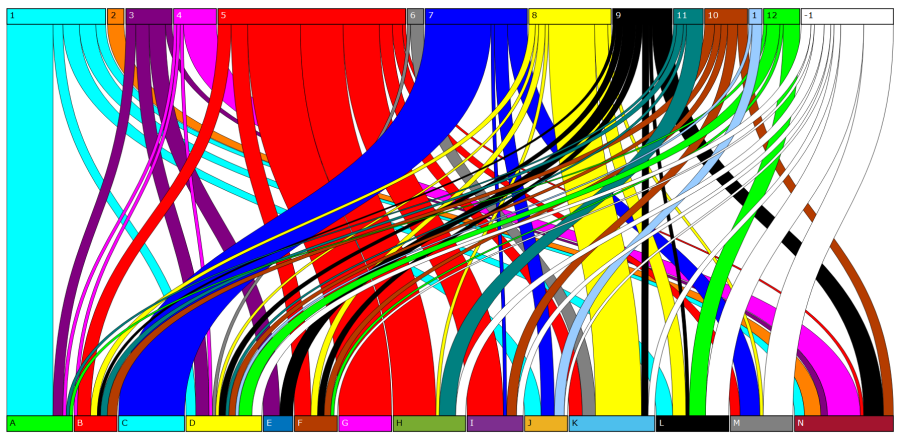
Most communities are spatially contiguous.

Block-structured solution

- SCD+Lasso selects 49 non-zero coefficients (out of 105)
- Default mode network (Power system 5) has been split into three (G, H, I), with different signs



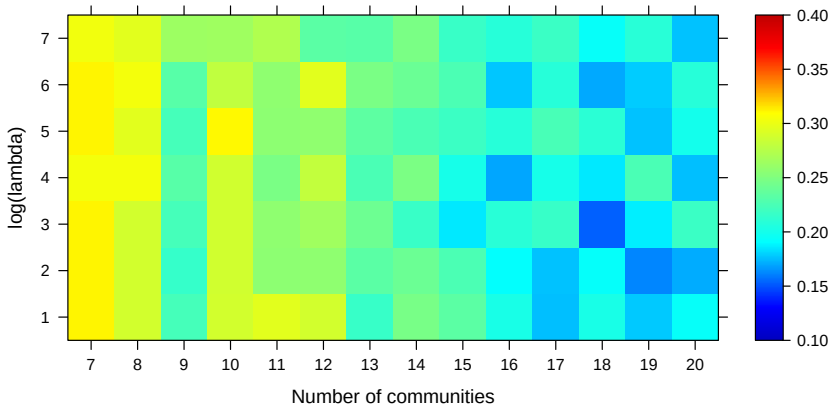
SCD: fitted coefficients



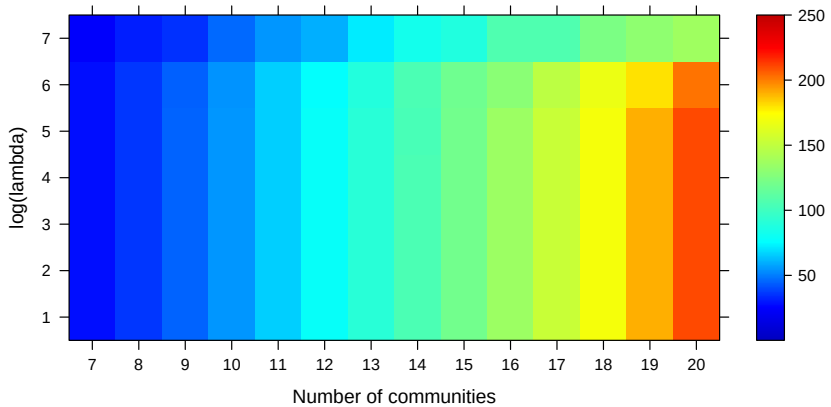
Sankey diagram:
Power (top) vs SCD (bottom)

Cross-validated prediction errors

Cross-validation error



Number of non-zero coefficients



Summary

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- Supervised communities simplify interpretation and provide more insights about the specific outcome variable
- Future work:
  - Extensions of the regularization to problems of interest
  - Valid statistical inference
  - Task-dependent brain regions in other relevant scenarios

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Thank you!

Arroyo, J., Levina, E. (2020). *"Simultaneous prediction and community detection for networks with application to neuroimaging"*, arXiv:2002.01645.

References I

- Aine, C. J. et al. (Oct. 2017). "Multimodal Neuroimaging in Schizophrenia: Description and Dissemination". In: *Neuroinformatics* 15.4, pp. 343–364.
- Arroyo Relión, Jesús D. et al. (Jan. 2019). "Network classification with applications to brain connectomics". In: *Annals of Applied Statistics* 13.3, pp. 1648–1677. arXiv: 1701.08140.
- Holland, Paul W., Kathryn Blackmond Laskey, and Samuel Leinhardt (June 1983). "Stochastic blockmodels: First steps". In: *Social Networks* 5.2, pp. 109–137.
- Power, Jonathan D et al. (2011). "Functional network organization of the human brain". In: *Neuron* 72.4, pp. 665–678.
- Priebe, Carey E et al. (2019). "On a two-truths phenomenon in spectral graph clustering". In: *Proceedings of the National Academy of Sciences* 116.13, pp. 5995–6000.