Collective Discovery of Brain Network with Unknown Groups

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Network Representation of Brain

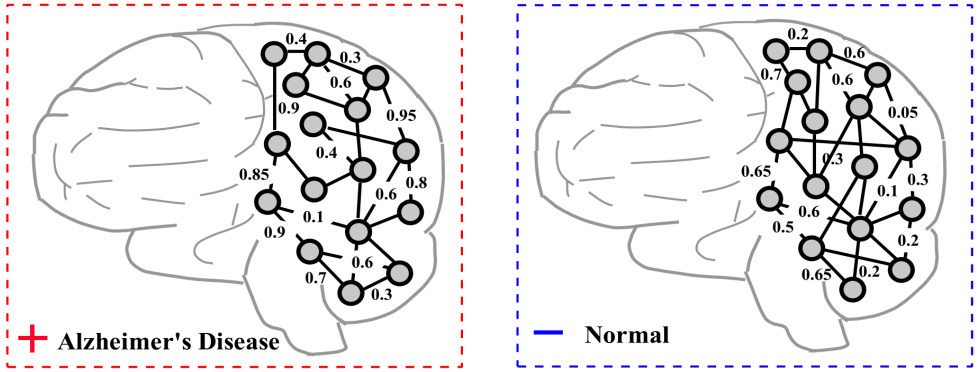
Each node = a brain region

Each edge = a functional connection

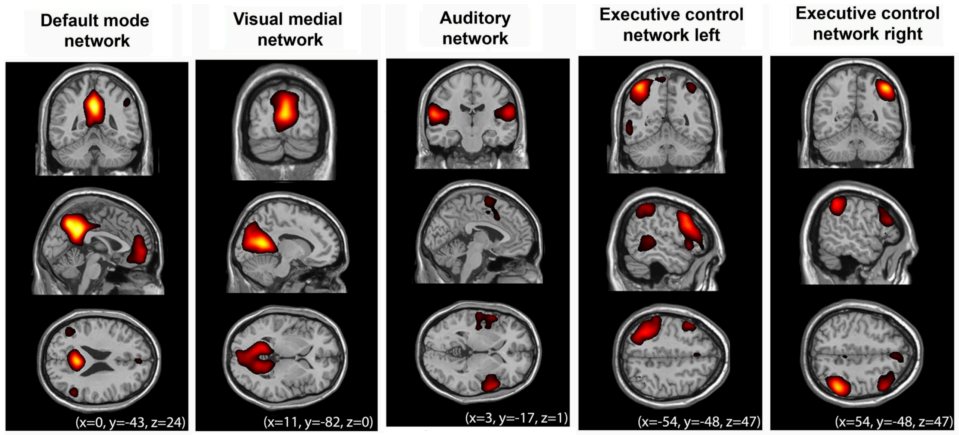
Use of Brain Network

Not Given!
Should be derived from neuroimaging data

Disease Diagnosis

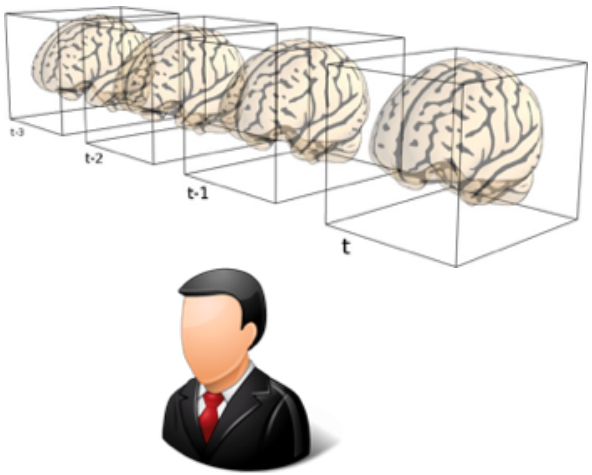


Functional Study



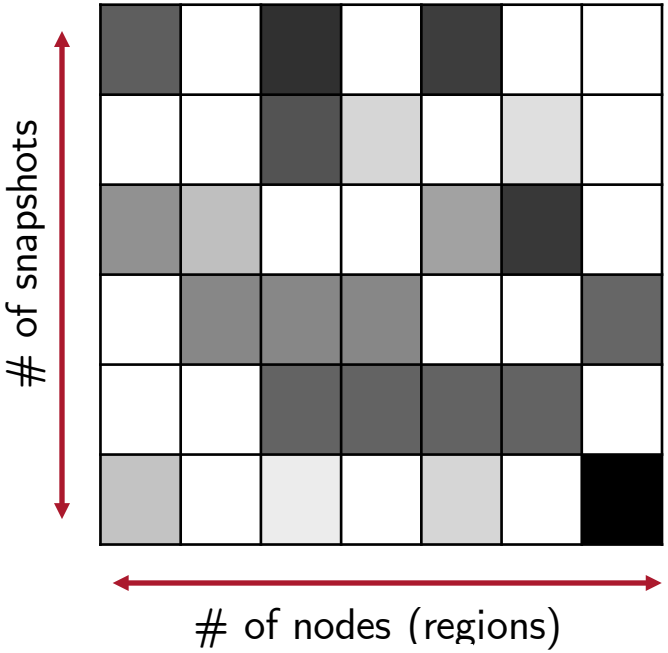
The fMRI Data

Each column refers to a voxel of the brain
Each row refers to a snapshot of the brain



The Data Matrix

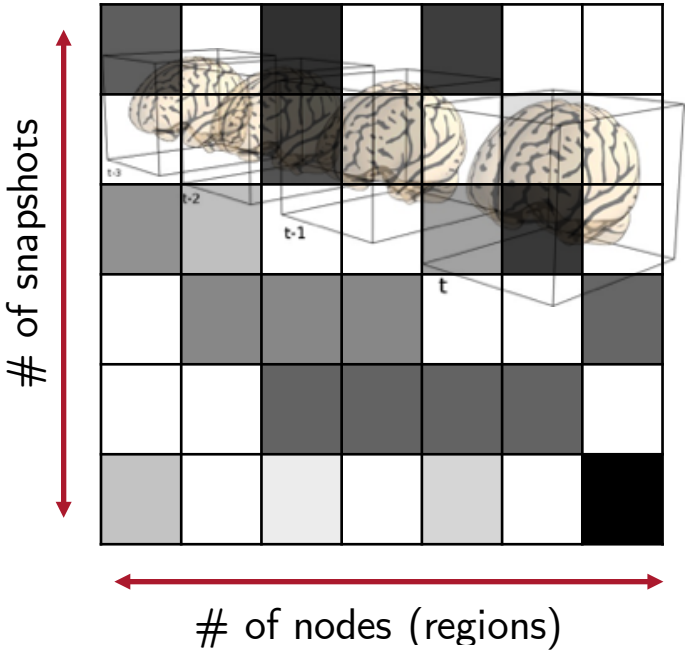
$X \in R^{m \times n}$



$\mathbf{X}$

Brain Network Discovery Problem

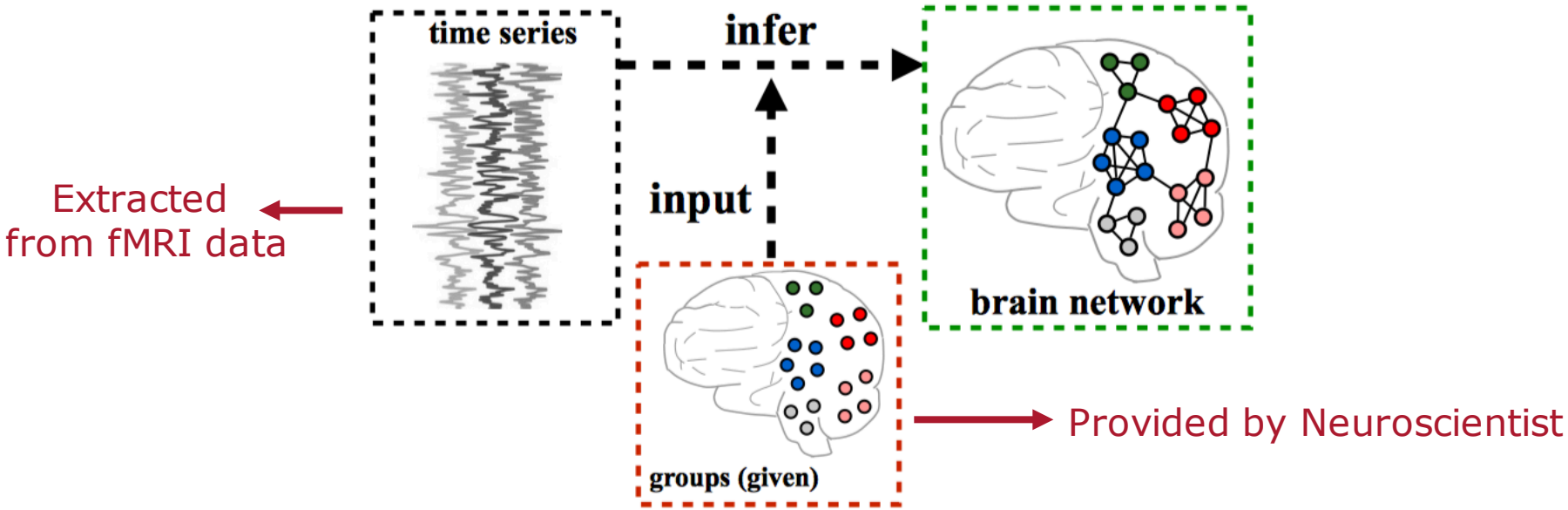
Input



$\mathbf{X}$

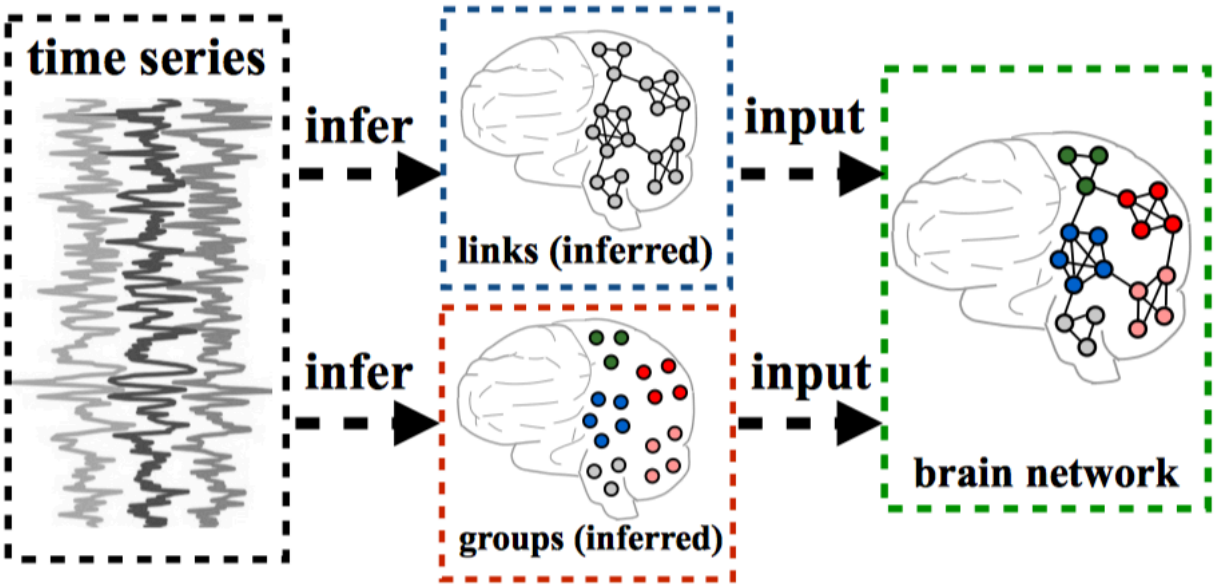
Output

Brain Network Discovery



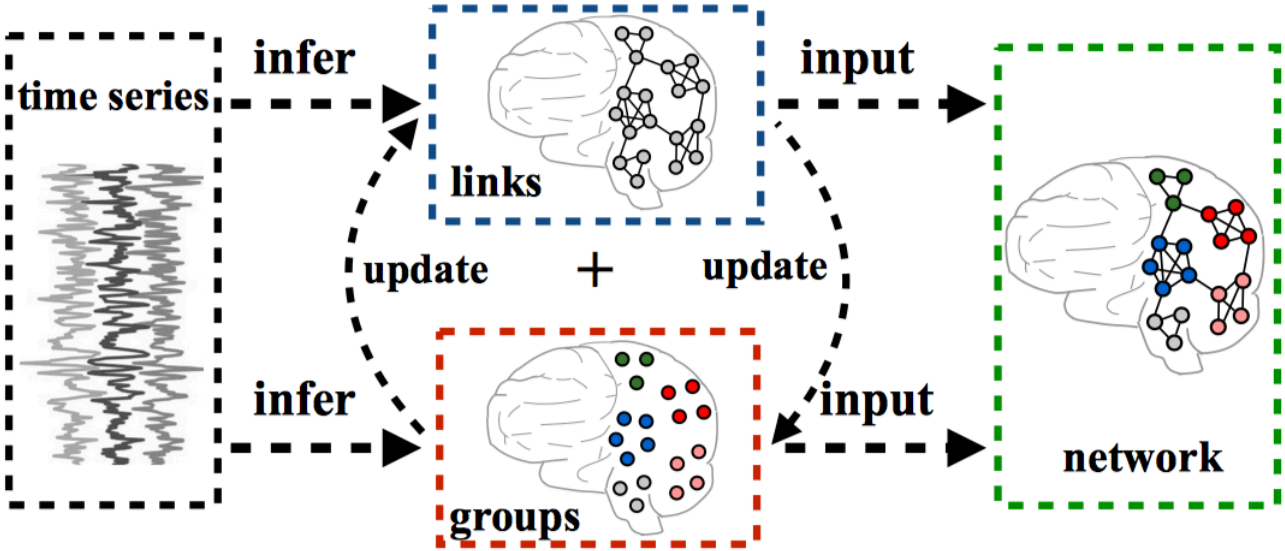
(a) Edge Inference with Known Groups

Brain Network Discovery Cont.



(b) Independent Inference

Collective Brain Network Discovery



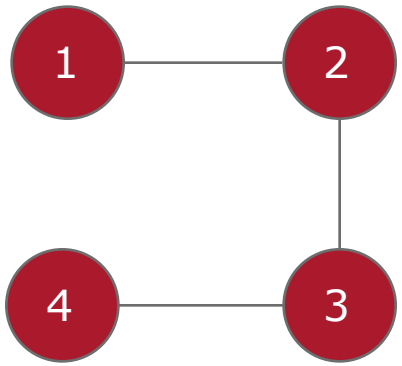
(c) Collective Inference (Proposed)

Why Collective?

- [Edge/Link]: The predefined groups may be inferred anatomically and contain sub-regions that are each characterized by different functional connectivity patterns.
- [Node/Group]: In most brain network inference model, once the groups (nodes) are derived, it is difficult or impossible to improve it based on edges/links discovered in latter stages.

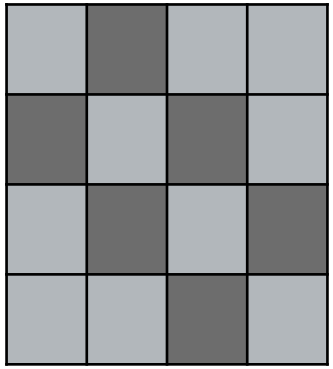
Preliminary: Inverse Covariance

Given time series signal of neurons



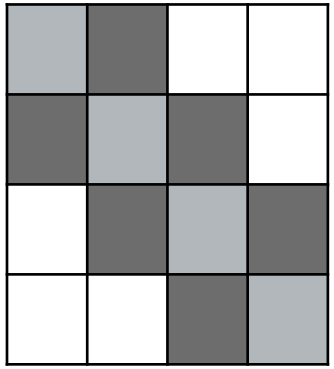
One can infer the connections between pairs of neurons using Pearson correlation

Covariance Matrix



Indirect Connections

Inverse Covariance Matrix



Direct Connections

Preliminary: Compute the Inverse

$$\boxed{\mathbf{S} = \frac{1}{n}\mathbf{X}^T\mathbf{X}}$$

empirical covariance matrix

Find the precision (inverse covariance) matrix

$$\boldsymbol{\Theta} \approx \mathbf{S}^{-1}$$

Very likely to be singular

Preliminary: Graphical Lasso

$$\underset{\boxed{\boldsymbol{\Theta} \succ 0}}{\text{minimize}} \quad \underbrace{-\log\det \boldsymbol{\Theta} + \mathrm{tr}(\mathbf{S}\boldsymbol{\Theta})}_{\text{Negative Log Likelihood}} + \underbrace{\lambda||\boldsymbol{\Theta}||_1}_{\text{L1-norm Regularization}}$$

positive definite constraint

Find a sparse positive definite matrix $\boldsymbol{\Theta}$ which has high likelihood to be the precision matrix of $\boldsymbol{S}$

SGGL Model: Step 1 (Group Constrained Graphical Lasso)

$$\underset{\boxed{\boldsymbol{\Theta} \succ 0}}{\arg\min} \underbrace{-\log\det\boldsymbol{\Theta} + \mathrm{tr}(\mathbf{S}\boldsymbol{\Theta})}_{\text{Negative Log Likelihood}} + \sum_{i,j} \underbrace{\lambda_{ij} ||\{\boldsymbol{\Theta}_{G_i,G_j}\}||_F}_{\text{Group-wise Sparseness Regularizer}}$$

positive definite constraint

Solved by Spectral Projected Gradient Descent

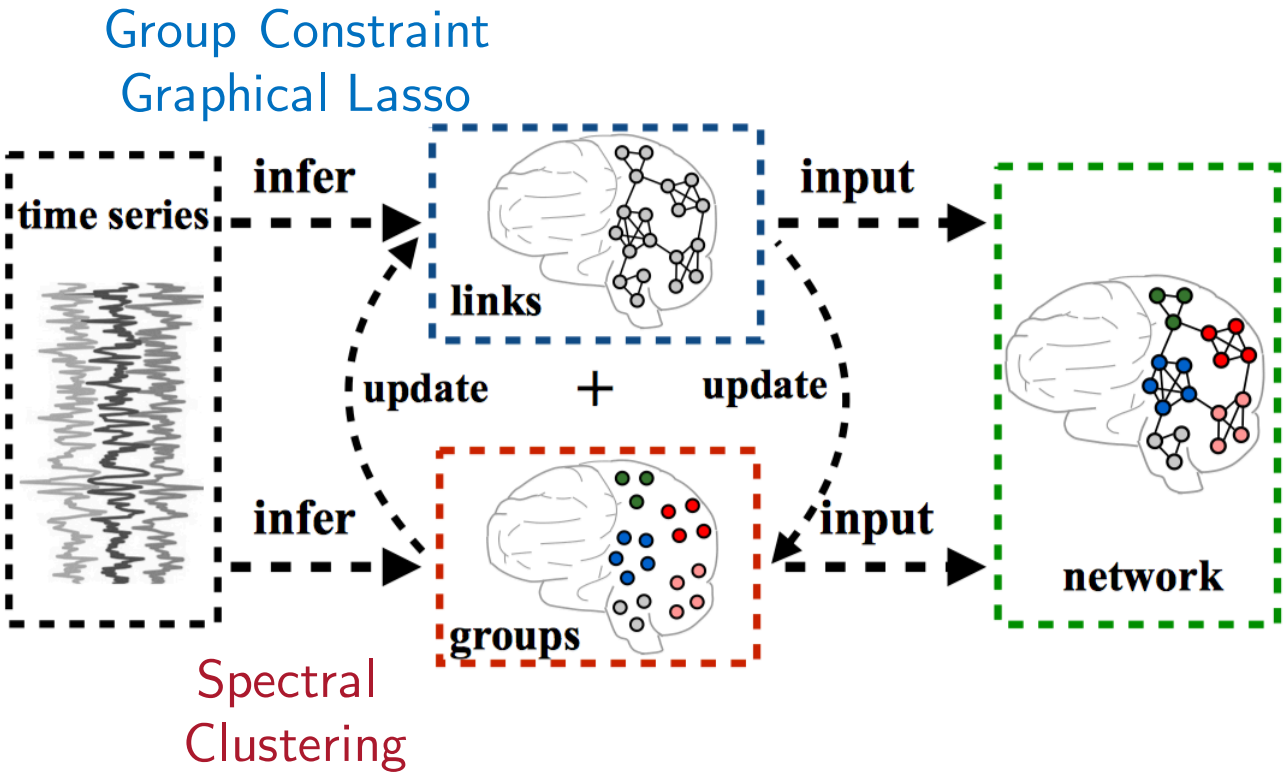
SGGL Model: Step 2 (Spectral Clustering)

use $\mathbf{\Omega}(\hat{\mathbf{\Theta}}) = \mathrm{abs}(\hat{\mathbf{\Theta}})$

as the affinity/similarity matrix for spectral clustering

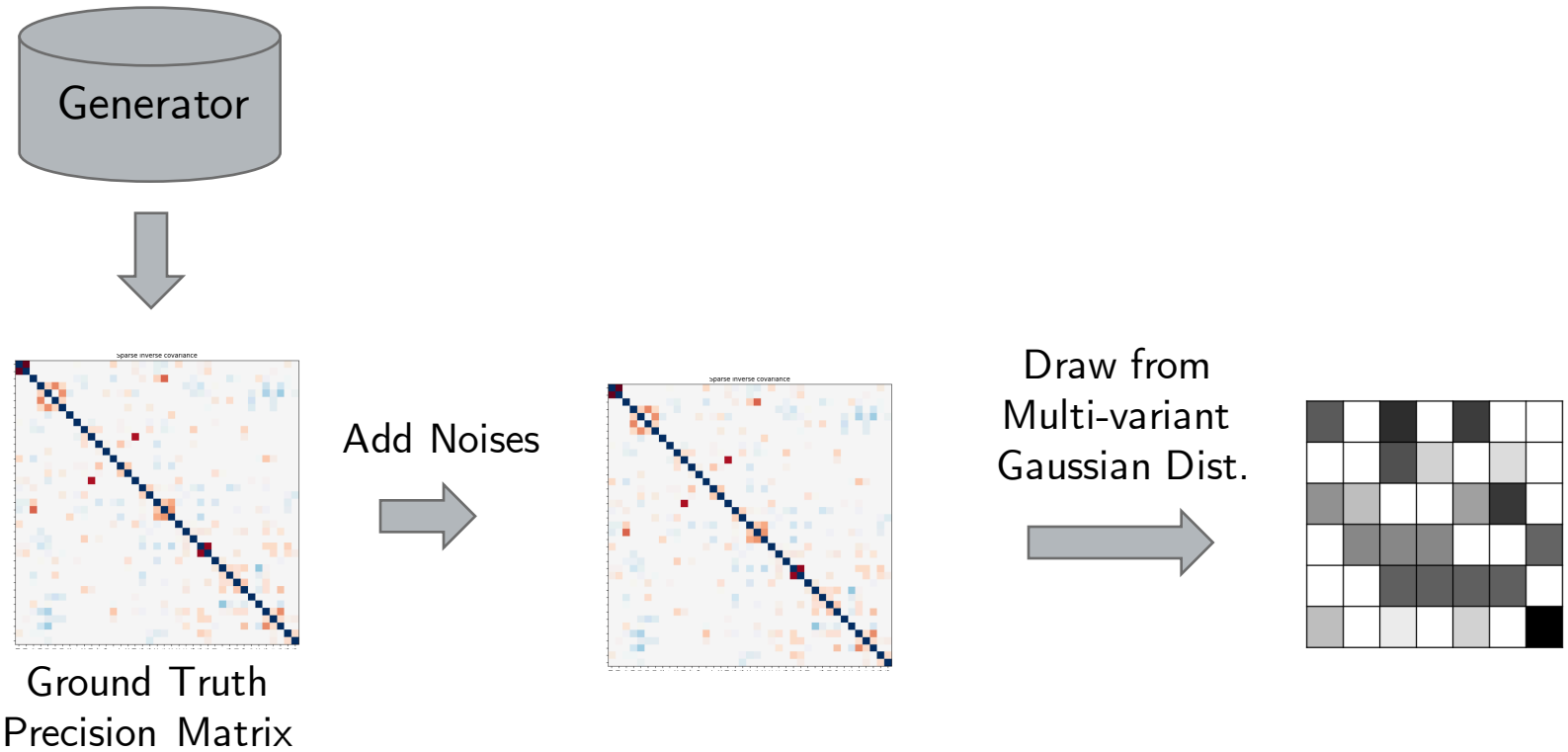
to update the group/node $(G_1,\ldots,G_N)$

SGGL Model: Iterative Inference



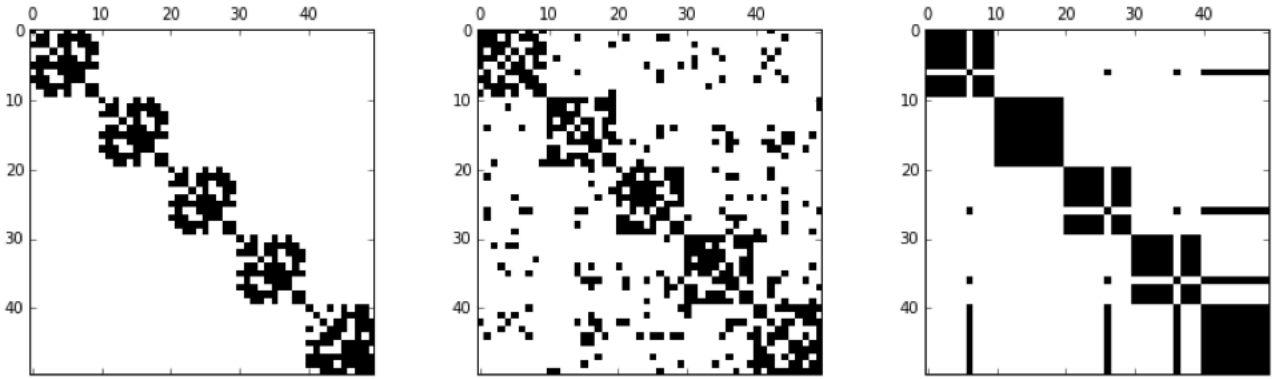
(c) Collective Inference (Proposed)

Synthetic Data



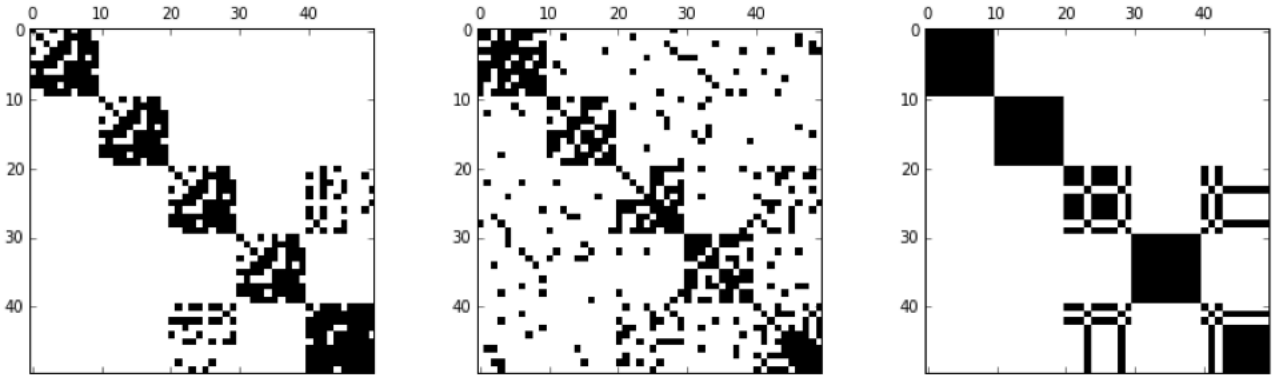
Synthetic Study (Illustration)

Data set 1



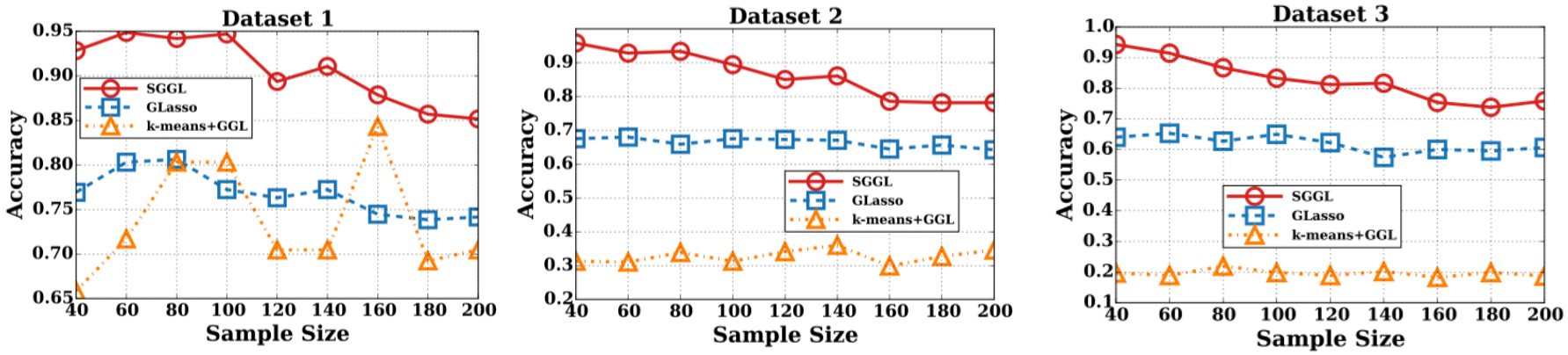
(a) Ground Truth (b) GLasso (c) SGGL

Data set 2



(d) Ground Truth (e) GLasso (f) SGGL

Synthetic Study (Edge Inference)

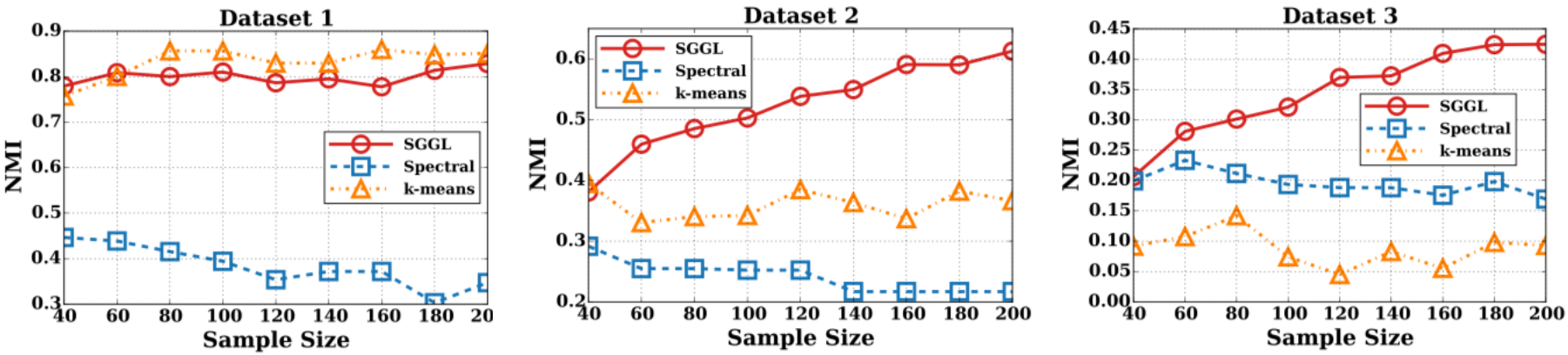


(a) Accuracy of Dataset 1 (b) Accuracy of Dataset 2 (c) Accuracy of Dataset 3

Compared Method:

- SGGL (proposed)
- Graphical Lasso
- K-means + GGL

Synthetic Study (Group Inference)



(a) NMI of Dataset 1 (b) NMI of Dataset 2 (c) NMI of Dataset 3

Compared Method:

- SGGL (proposed)
- Spectral Clustering
- K-means

Real fMRI Data

- ADHD-200
  - 20 healthy (TDC) subjects, 20 ADHD patients.
  - 3D brain images of size 61 x 73 x 61 ~ 180 time steps

- All parameters are tuning using DMN.

Real fMRI data (DMN Recovery)

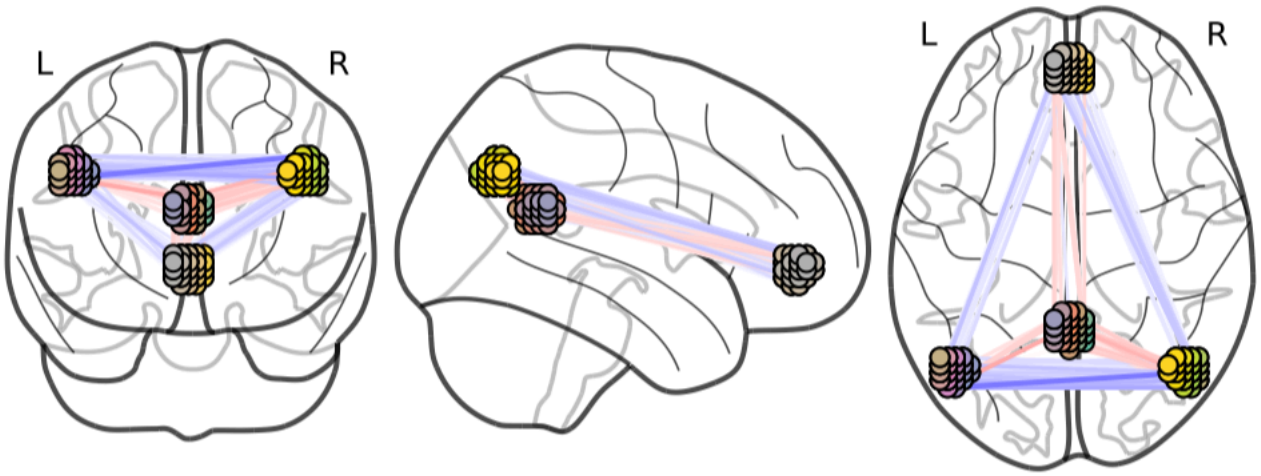


Fig. 7. The connectivity of DMN of ADHD group discovered by SGGL. All regions in the DMN are strongly connected to each other, which is consistent with the essence of DMN.

Real fMRI data (DMN Recovery)

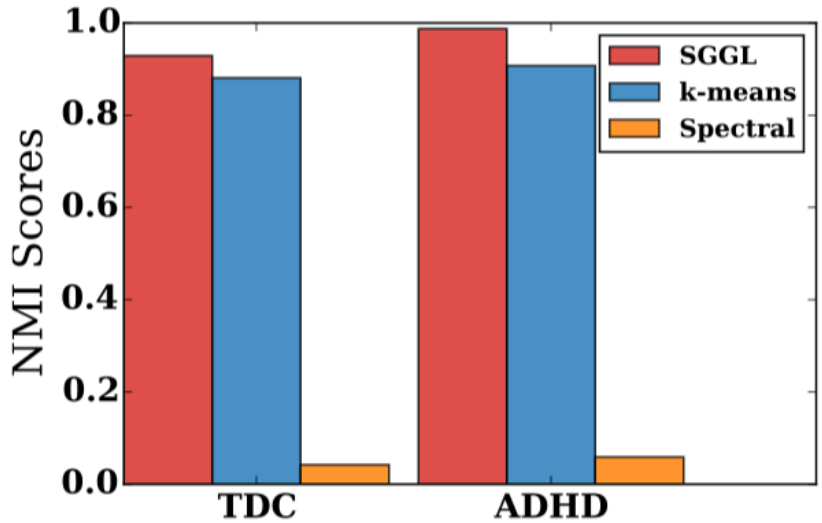
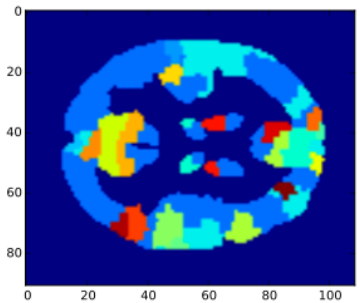


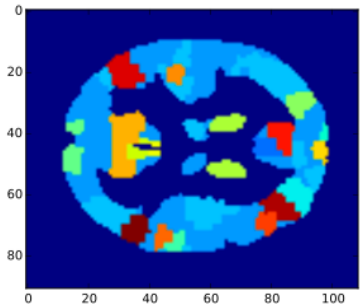
Fig. 6. Comparison of NMI scores on the DMN (Default Mode Network) of ADHD-200 Data.

Real fMRI data (Entire Brain Group Inference)

more Interpretable results

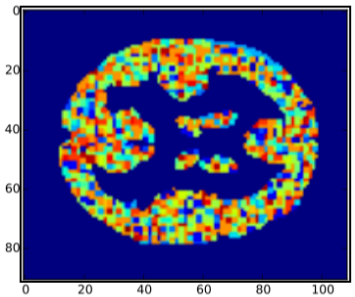


(a) Groups of TDC inferred by SGGL ($k = 20$)

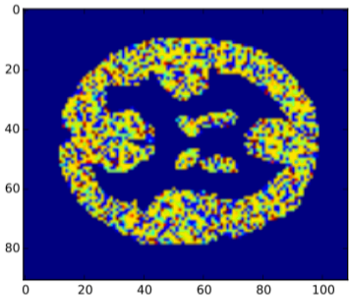


(b) Groups of ADHD inferred by SGGL ($k = 20$)

Scattered, hard to see difference

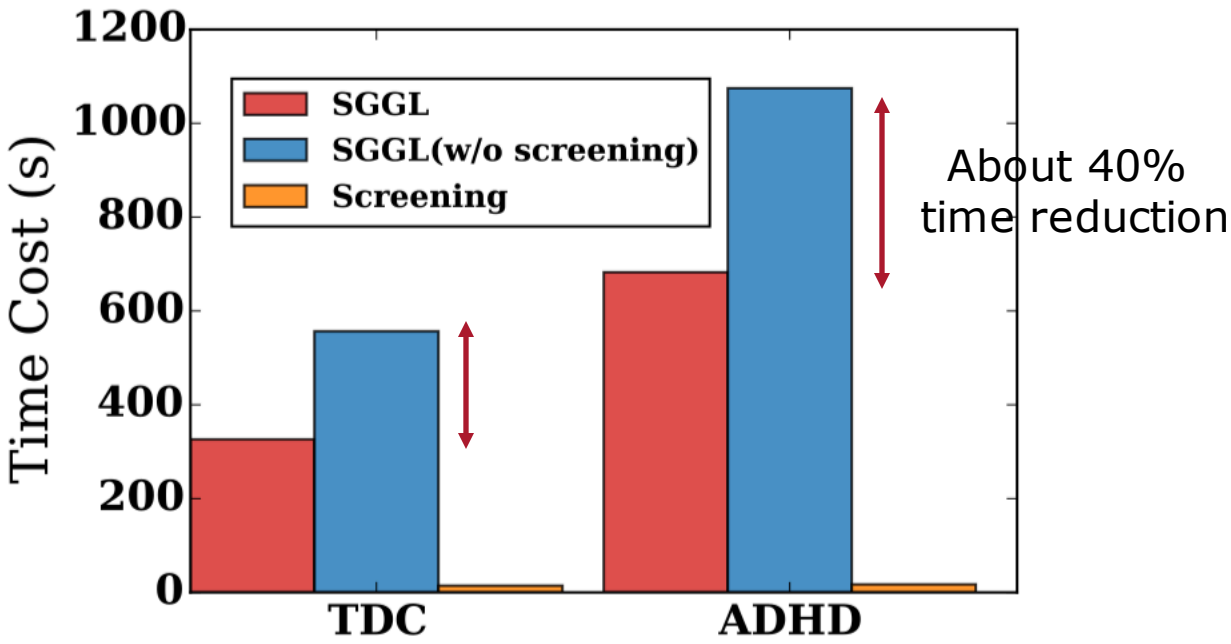


(c) Groups of TDC inferred by spectral clustering ($k = 20$)



(d) Groups of ADHD inferred by spectral clustering ($k = 20$)

Effect of Screening



Summary

- Problem Studied
  - Collective brain network discovery (nodes + edges)
- Proposed solution
  - Use Group Constrained Graphical Lasso to infer the edges
  - Use spectral clustering with the masked precision matrix as the affinity matrix to update the group
  - Use the updated group to further update the edges and to repeat previous two steps until converge
  - A set of screening rules is proposed to speed up the edge inference
- Conclusion
  - Experiments on synthetic data and real-world fMRI demonstrated the superiority of the proposed SGGL method

Q&A

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