

Online Topology Inference from Streaming Stationary Graph Signals

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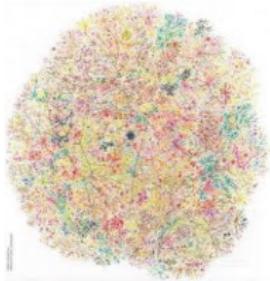
IEEE Data Science Workshop, June 4, 2019

Network Science analytics

Online social media



Internet



Clean energy and grid analytics



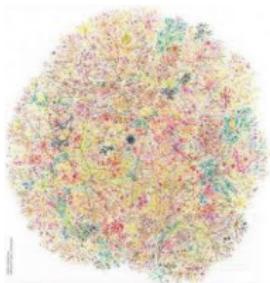
- Network as graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$: encode pairwise relationships
- Desiderata: Process, analyze and learn from network data [Kolaczyk'09]

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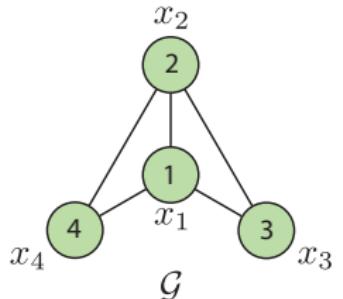
Clean energy and grid analytics



- Network as graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$: encode pairwise relationships
- Desiderata: Process, analyze and learn from network data [Kolaczyk'09]
- Interest here not in \mathcal{G} itself, but in data associated with nodes in \mathcal{V}
 ⇒ The object of study is a graph signal
- Ex: Opinion profile, buffer congestion levels, neural activity, epidemic

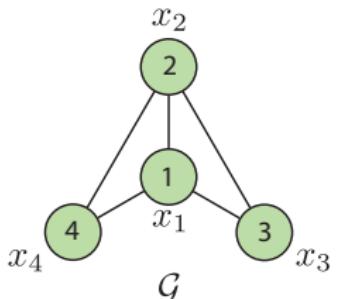
Graph signal processing (GSP)

- ▶ Undirected \mathcal{G} with **adjacency matrix \mathbf{A}**
 $\Rightarrow A_{ij} = \text{Proximity between } i \text{ and } j$
- ▶ Define a **signal \mathbf{x}** on top of the graph
 $\Rightarrow x_i = \text{Signal value at node } i$



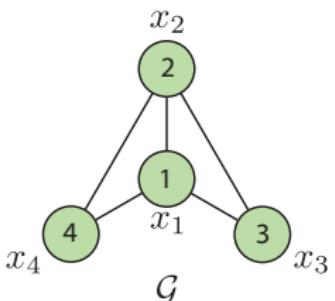
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- ▶ Define a signal \mathbf{x} on top of the graph
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- ▶ Associated with \mathcal{G} is the graph-shift operator (GSO) $\mathbf{S} = \mathbf{V}\Lambda\mathbf{V}^T \in \mathcal{M}^N$
 $\Rightarrow S_{ij} = 0$ for $i \neq j$ and $(i,j) \notin \mathcal{E}$ (local structure in G)
 \Rightarrow Ex: \mathbf{A} , degree \mathbf{D} and Laplacian $\mathbf{L} = \mathbf{D} - \mathbf{A}$ matrices



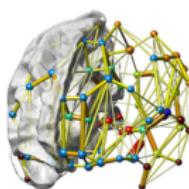
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 \Rightarrow Ex: **\mathbf{A}** , degree **\mathbf{D}** and Laplacian **$\mathbf{L} = \mathbf{D} - \mathbf{A}$** matrices
- ▶ **Graph Signal Processing** \rightarrow Exploit structure encoded in **\mathbf{S}** to process **\mathbf{x}**
 \Rightarrow GSP well suited to study (network) diffusion processes
- ▶ Use GSP to learn the underlying \mathcal{G} or a meaningful network model



Topology inference: Motivation and context

- ▶ Network **topology inference** from nodal observations [Kolaczyk'09]
 - ▶ Partial correlations and conditional dependence [Dempster'74]
 - ▶ Sparsity [Friedman et al'07] and consistency [Meinshausen-Buhlmann'06]
 - ▶ [Banerjee et al'08], [Lake et al'10], [Slawski et al'15], [Karanikolas et al'16]
- ▶ Can be useful in neuroscience [Sporns'10]
 - ⇒ Functional net inferred from activity
- ▶ Noteworthy **GSP**-based approaches
 - ▶ Gaussian graphical models [Egilmez et al'16]
 - ▶ Smooth signals [Dong et al'15], [Kalofolias'16]
 - ▶ Stationary signals [Pasdeloup et al'15], [Segarra et al'16]
 - ▶ Non-stationary signals [Shafipour et al'17]
 - ▶ Directed graphs [Mei-Moura'15], [Shen et al'16]
 - ▶ Low-rank excitation [Wai et al'18]
 - ▶ Learning from sequential data [Vlaski et al'18]
- ▶ **Here:** online topology inference from streaming **stationary** graph signals



Generating structure of a diffusion process

- ▶ Signal \mathbf{y} is the response of a linear diffusion process to an input \mathbf{x}

$$\mathbf{y} = \alpha_0 \prod_{l=1}^{\infty} (\mathbf{I} - \alpha_l \mathbf{S}) \mathbf{x} = \sum_{l=0}^{\infty} \beta_l \mathbf{S}^l \mathbf{x}$$

⇒ Common generative model. Heat diffusion if α_k constant

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⇒ Common generative model. Heat diffusion if α_k constant

- ▶ One can state that the graph shift \mathbf{S} explains the structure of signal \mathbf{y}
- ▶ Cayley-Hamilton asserts that we can write diffusion as

$$\mathbf{y} = \left(\sum_{l=0}^{L-1} h_l \mathbf{S}^l \right) \mathbf{x} := \mathcal{H}(\mathbf{S}) \mathbf{x} := \mathbf{H} \mathbf{x}$$

⇒ Degree $L \leq N$ depends on the dependency range of the filter

⇒ Shift invariant operator \mathbf{H} is graph filter [Sandryhaila-Moura'13]

- ▶ Online topology inference: From $\mathcal{Y} = \{\mathbf{y}^{(1)}, \dots, \mathbf{y}^{(P)}, \dots\}$, Find \mathbf{S} efficiently

Topology inference under stationarity

Stationary graph signal [Marques et al'16]

Def: A graph signal \mathbf{y} is stationary with respect to the shift \mathbf{S} if and only if $\mathbf{y} = \mathbf{H}\mathbf{x}$, where $\mathbf{H} = \sum_{l=0}^{L-1} h_l \mathbf{S}^l$ and \mathbf{x} is white.

- The covariance matrix of the **stationary** signal \mathbf{y} is

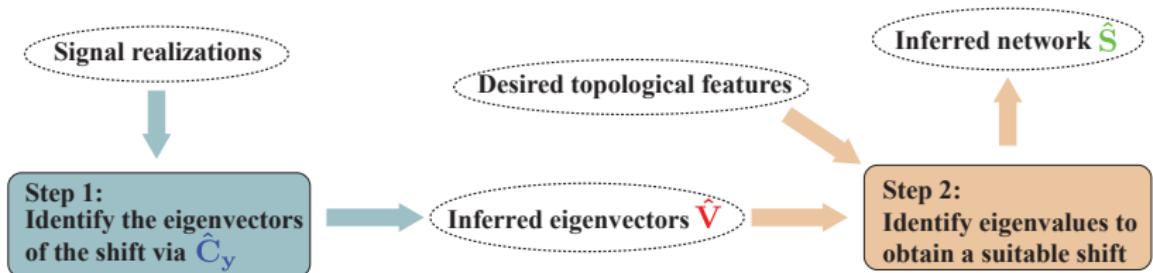
$$\mathbf{C}_y = \mathbb{E} \left[\mathbf{H}\mathbf{x} (\mathbf{H}\mathbf{x})^T \right] = \mathbf{H} \mathbb{E} \left[\mathbf{x}\mathbf{x}^T \right] \mathbf{H}^T = \mathbf{H}\mathbf{H}^T$$

- **Key:** Since \mathbf{H} is diagonalized by \mathbf{V} , so is the covariance \mathbf{C}_y

$$\mathbf{C}_y = \mathbf{V} \left| \sum_{l=0}^{L-1} h_l \Lambda^l \right|^2 \mathbf{V}^T = \mathbf{V} (\mathcal{H}(\Lambda))^2 \mathbf{V}^T$$

⇒ Estimate \mathbf{V} from \mathcal{Y} via Principal Component Analysis

Two-step approach [Segarra et al'17]



- ▶ Step 2: Obtaining the eigenvalues of \mathbf{S}
- ▶ We can use extra knowledge/assumptions to choose one graph
 - ⇒ Of all graphs, select one that is optimal in the number of edges

$$\hat{\mathbf{S}} := \underset{\mathbf{S}, \Lambda}{\operatorname{argmin}} \quad \|\mathbf{S}\|_1 \quad \text{subject to:} \quad \|\mathbf{S} - \hat{\mathbf{V}}\Lambda\hat{\mathbf{V}}^T\|_F \leq \epsilon, \quad \mathbf{S} \in \mathcal{S}$$

- ▶ Set \mathcal{S} contains all admissible scaled adjacency matrices

$$\mathcal{S} := \{\mathbf{S} \mid S_{ij} \geq 0, \quad \mathbf{S} \in \mathcal{M}^N, \quad S_{ii} = 0, \quad \sum_j S_{1j} = 1\}$$

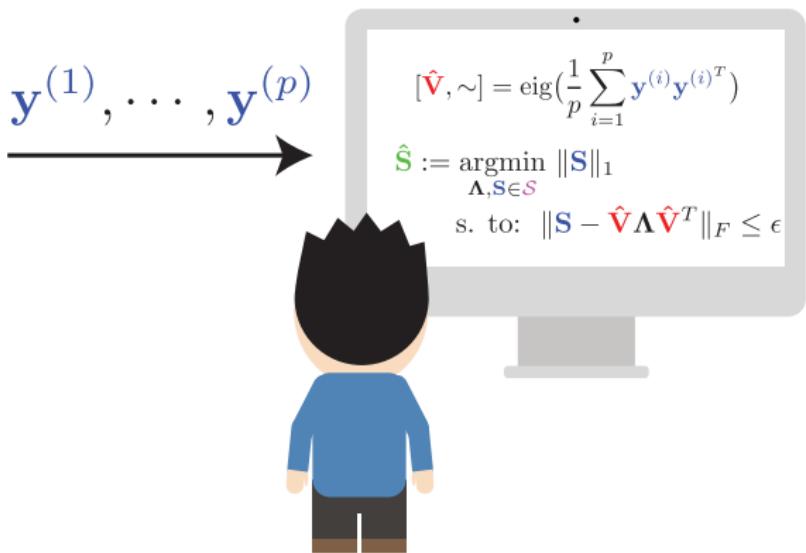


Online inference under stationarity

- ▶ Consider **streaming stationary** signals $\mathcal{Y} := \{\mathbf{y}^{(1)}, \dots, \mathbf{y}^{(p)}, \mathbf{y}^{(p+1)}, \dots\}$
- ▶ Assume that **time differences of the signals arrival** is relatively low

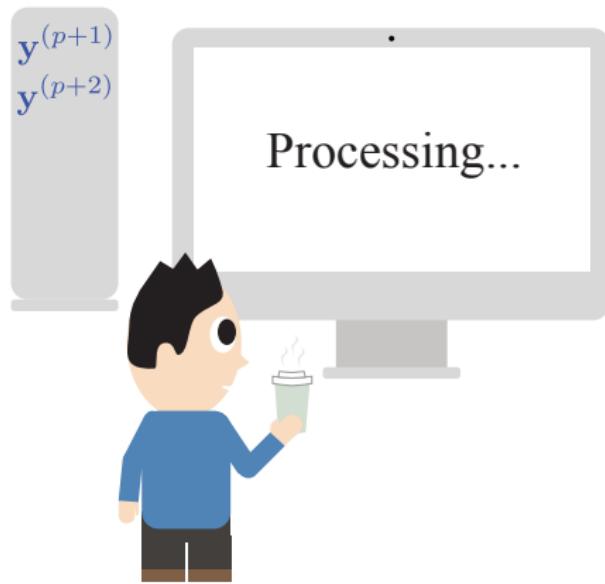
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- Develop an iterative algorithm for the topology inference
- Upon sensing new diffused output signals
 - ⇒ - Update $\hat{\mathbf{V}}$ efficiently
 - Take one or a few steps of the iterative algorithm



Topology inference via ADMM

- To apply ADMM, rewrite the problem as

$$\min_{\mathbf{S}, \mathbf{\Lambda}, \mathbf{D}} \quad \lambda \|\mathbf{S}\|_1 + \|\mathbf{S} - \hat{\mathbf{V}} \mathbf{\Lambda} \hat{\mathbf{V}}^\top\|_F^2$$

s.to: $\mathbf{S} - \mathbf{D} = \mathbf{0}$, $\mathbf{D} \in \mathcal{S} = \{\mathbf{S} \mid S_{ij} \geq 0, \mathbf{S} \in \mathcal{M}^N, S_{ii} = 0, \sum_j S_{1j} = 1\}$

\Rightarrow Convex, thus ADMM would converge to a global minimizer

- Form the augmented Lagrangian

$$\mathcal{L}_{\rho_1}(\mathbf{S}, \mathbf{D}, \mathbf{\Lambda}, \mathbf{U}_1) = \lambda \|\mathbf{S}\|_1 + \|\mathbf{S} - \hat{\mathbf{V}} \mathbf{\Lambda} \hat{\mathbf{V}}^\top\|_F^2 + \frac{\rho_1}{2} \|\mathbf{S} - \mathbf{D} + \mathbf{U}_1\|_F^2$$

- At k^{th} iteration, let $\mathbf{B}^{(k)} = \hat{\mathbf{V}} \mathbf{\Lambda}^{(k)} \hat{\mathbf{V}}^\top \Rightarrow$ ADMM consists of 4 iterative steps

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- Step 1.** $\mathbf{S}^{(k+1)} = \underset{\mathbf{S}}{\operatorname{argmin}} \mathcal{L}_{\rho_1}(\mathbf{S}, \mathbf{D}^{(k)}, \boldsymbol{\Lambda}^{(k)}, \mathbf{U}_1^{(k)}) = \mathcal{T}_{\frac{\lambda}{2+\rho_1}}\left(\frac{\mathbf{B}^{(k)} + \frac{\rho_1}{2}(\mathbf{D}^{(k)} - \mathbf{U}_1^{(k)})}{1 + \frac{\rho_1}{2}}\right)$,
where $\mathcal{T}_\eta(x) = (|x| - \eta)_+ \operatorname{sign}(x)$ is the element-wise soft-thresholding operator

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- Step 2.** $\mathbf{D}^{(k+1)} = \underset{\mathbf{D} \in \mathcal{S}}{\operatorname{argmin}} \quad \mathcal{L}_{\rho_1}(\mathbf{S}^{(k+1)}, \mathbf{D}, \mathbf{\Lambda}^{(k)}, \mathbf{U}_1^{(k)}) = \mathcal{P}_{\mathcal{S}}(\mathbf{S}^{(k+1)} + \mathbf{U}_1^{(k)}),$
where $\mathcal{P}_{\mathcal{S}}(\cdot)$ is the projection operator onto \mathcal{S}

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- At k^{th} iteration, let $\mathbf{B}^{(k)} = \hat{\mathbf{V}} \boldsymbol{\Lambda}^{(k)} \hat{\mathbf{V}}^\top \Rightarrow$ ADMM consists of 4 iterative steps
- Step 3.** $\boldsymbol{\Lambda}^{(k+1)} = \underset{\boldsymbol{\Lambda}}{\operatorname{argmin}} \quad \mathcal{L}_{\rho_1}(\mathbf{S}^{(k+1)}, \mathbf{D}^{(k+1)}, \boldsymbol{\Lambda}, \mathbf{U}_1^{(k)})$

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- At k^{th} iteration, let $\mathbf{B}^{(k)} = \hat{\mathbf{V}} \mathbf{\Lambda}^{(k)} \hat{\mathbf{V}}^\top \Rightarrow$ ADMM consists of 4 iterative steps
- Step 4.** Dual gradient ascent update $\mathbf{U}_1^{(k+1)} = \mathbf{U}_1^{(k)} + \mathbf{S}^{(k+1)} - \mathbf{D}^{(k+1)}$

Topology inference algorithm

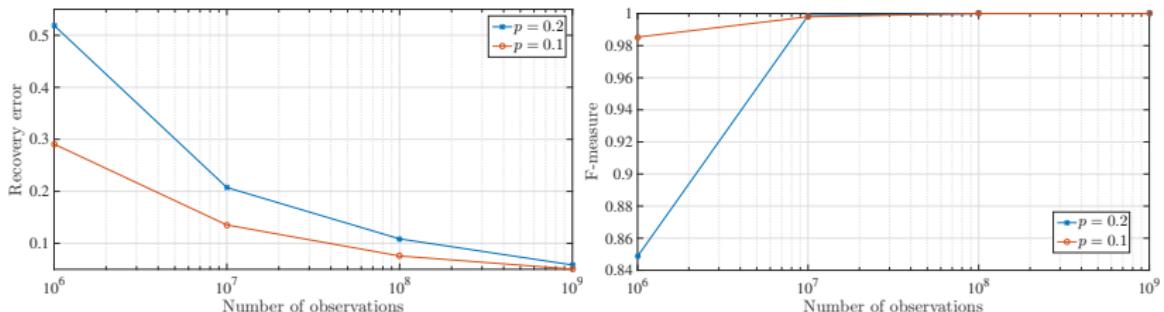
- 1: **Input:** estimated covariance eigenvectors $\hat{\mathbf{V}}$, penalty parameter ρ_1 , regularization parameter λ , number of iterations T_1
- 2: **Initialize:** $\Lambda^{(0)} = \text{diag}(\mathbf{1}_N)$, $\mathbf{D}^{(0)} = \mathbf{0}$, $\mathbf{U}_1^{(0)} = \mathbf{0}$.
- 3: **for** $k = 0, \dots, T_1 - 1$ **do**
- 4: $\mathbf{B}^{(k)} = \hat{\mathbf{V}} \Lambda^{(k)} \hat{\mathbf{V}}^\top$
- 5: $\mathbf{S}^{(k+1)} = \mathcal{T}_{\frac{\lambda}{2+\rho_1}}\left(\frac{\mathbf{B}^{(k)} + \frac{\rho_1}{2}(\mathbf{D}^{(k)} - \mathbf{U}_1^{(k)})}{1 + \frac{\rho_1}{2}}\right)$
- 6: $\mathbf{D}^{(k+1)} = \mathcal{P}_{\mathcal{S}}(\mathbf{S}^{(k+1)} + \mathbf{U}_1^{(k)})$
- 7: $\Lambda^{(k+1)} = \text{Diag}(\hat{\mathbf{V}}^\top \mathbf{S}^{(k+1)} \hat{\mathbf{V}})$
- 8: $\mathbf{U}_1^{(k+1)} = \mathbf{U}_1^{(k)} + \mathbf{S}^{(k+1)} - \mathbf{D}^{(k+1)}$
- 9: **end for**
- 10: **return** $\mathbf{S}^{(T_1)}$ and $\Lambda^{(T_1)}$

- Develop an iterative algorithm for the topology inference
- Upon sensing new diffused output signals
 - ⇒ - Update Λ efficiently
 - Take one or a few steps of the iterative algorithm



Inferring a large scale graph

- ▶ Consider an Erdős-Rényi graph with $N=1000$ in an offline fashion
 - ▶ Edges are formed independently with probabilities $p=0.1$ & 0.2
 - ▶ Signals diffused by $\mathbf{H} = \sum_{l=0}^2 h_l \mathbf{A}^l$, $h_l \sim \mathcal{U}[0, 1]$, $\mathbf{S} = \mathbf{A}$
 - ▶ Adopt sample covariance estimator for the Gaussian signals
 - ▶ Assess the recovery error $\xi_F := \|\hat{\mathbf{S}} - \mathbf{S}\|_F / \|\mathbf{S}\|_F$ and F-measure



- ▶ Increase in **number of observations** leads to a better performance
 - ⇒ Performance enhances for **sparser** graphs (i.e., smaller p)

Online topology inference

- **Q:** How can we **efficiently** update the sample covariance eigenvectors $\hat{\mathbf{V}}$?

- Let $\hat{\mathbf{C}}_{\mathbf{y}}^{(P)}$ be sample covariance after receiving P streaming observations
 \Rightarrow Updated sample covariance after receiving $\mathbf{y}^{(P+1)}$ takes the form

$$\hat{\mathbf{C}}_{\mathbf{y}}^{(P+1)} = \frac{1}{P+1} (P \hat{\mathbf{C}}_{\mathbf{y}}^{(P)} + \mathbf{y}^{(P+1)} \mathbf{y}^{(P+1)^\top})$$

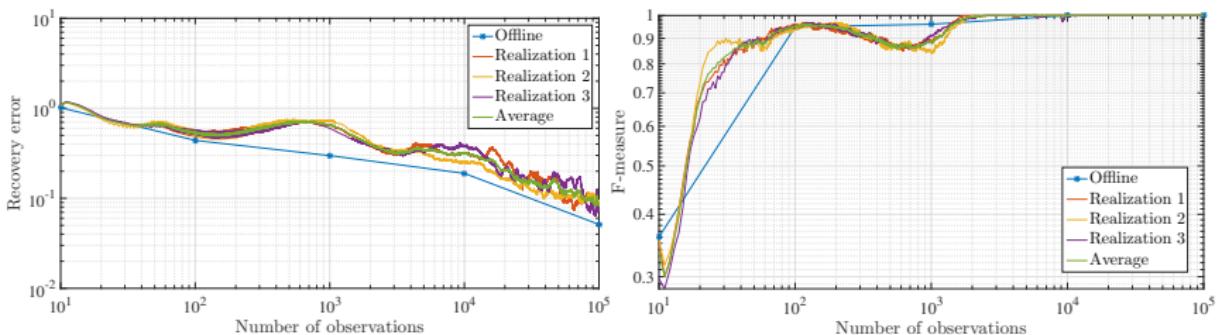
- Let $\mathbf{z} = \hat{\mathbf{V}}^\top \mathbf{y}^{(P+1)}$ and $\{d_j\}_{j=1}^N$ denote the **eigenvalues** of $\hat{\mathbf{C}}_{\mathbf{y}}^{(P)}$
 \Rightarrow Eigenvalues of rank-one modification of $\hat{\mathbf{C}}_{\mathbf{y}}^{(P)}$ are the roots (γ) of
$$1 + \sum_{j=1}^N \frac{\mathbf{z}_j^2}{P d_j - \gamma} = 0 \quad [\text{Bunch et al'78}]$$
 \Rightarrow Can be solved using the **Newton** method with $\mathcal{O}(N^2)$ complexity
- For the updated eigenvalue γ_j , the corresponding eigenvector \mathbf{v}_j is given by

$$\mathbf{v}_j = \alpha_j \mathbf{y}^{(P+1)} \circ \mathbf{q}_j,$$

where $\mathbf{q}_j = [1/(P d_1 - \gamma_j), \dots, 1/(P d_N - \gamma_j)]$ and α_j is a normalizing factor

Online inference of a brain network

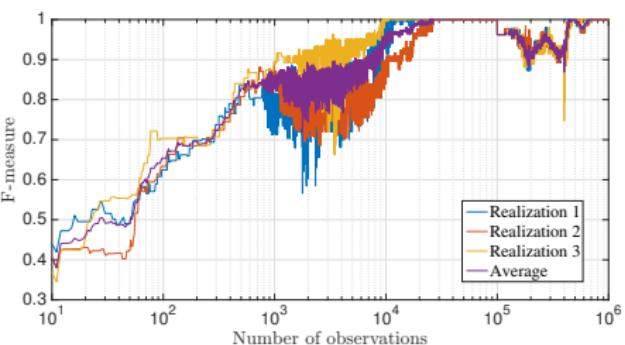
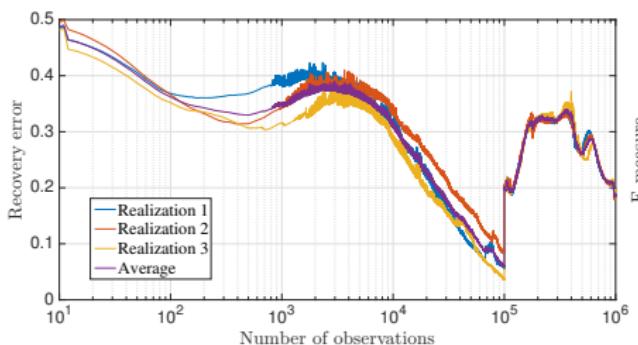
- ▶ Consider a **structural brain graph** with $N = 66$ neural regions
 - ▶ Edge weights: Density of anatomical connections [Hagmann et al'08]
 - ▶ Signals diffused by $\mathbf{H} = \sum_{l=0}^2 h_l \mathbf{A}^l$, $h_l \sim \mathcal{U}[0, 1]$, $\mathbf{S} = \mathbf{A}$
 - ▶ Generate streaming signals $\{\mathbf{y}^{(1)}, \dots, \mathbf{y}^{(p)}, \mathbf{y}^{(p+1)}, \dots\}$ via $\mathbf{y}^{(i)} = \mathbf{Hx}^{(i)}$
 - ▶ Upon sensing an observation $\mathbf{y}^{(p)}$
 - ⇒ Update $\hat{\mathbf{V}}$ efficiently and run the algorithm for $T_1 = 1$
 - ▶ Assess the recovery error $\xi_F := \|\hat{\mathbf{S}} - \mathbf{S}\|_F / \|\mathbf{S}\|_F$ and F-measure



- ▶ The **online** scheme can track the performance of the **batch** inference
 - ⇒ The fluctuations are due to **ADMM** and **online** scheme

Online inference: Synthetic perturbation

- ▶ Consider an Erdős-Renyi graph with $N=20$ and $p=0.2$
 - ▶ Signals diffused by $\mathbf{H} = \sum_{l=0}^2 h_l \mathbf{A}^l$, $h_l \sim \mathcal{U}[0, 1]$, $\mathbf{S} = \mathbf{A}$
 - ▶ Generate streaming signals $\{\mathbf{y}^{(1)}, \dots, \mathbf{y}^{(p)}, \mathbf{y}^{(p+1)}, \dots\}$ via $\mathbf{y}^{(i)} = \mathbf{Hx}^{(i)}$
 - ▶ Upon sensing an observation $\hat{\mathbf{V}}$
 \Rightarrow Update $\hat{\mathbf{V}}$ efficiently and run the algorithm for $T_1=1$
 - ▶ After 10^5 realizations
 \Rightarrow Remove 10% of edges and add the same number of edges elsewhere
 - ▶ Assess the recovery error $\xi_F := \|\hat{\mathbf{S}} - \mathbf{S}\|_F / \|\mathbf{S}\|_F$ and F-measure



- ▶ The online algorithm can adapt and learn the new topology

Closing remarks

- ▶ Online topology inference from streaming stationary graph signals
 - ▶ Graph shift \mathbf{S} and covariance \mathbf{C}_y are simultaneously diagonalizable
 - ▶ Promote desirable properties via convex losses on $\mathbf{S} \Rightarrow$ Here: Sparsity

- Developed an iterative algorithm for the topology inference
- Upon sensing new diffused output signals
 ⇒ - Updated $\hat{\mathbf{V}}$ efficiently
 - Took one or a few steps of the iterative algorithm



Back to the \mathbf{D} -update

- Recall **Step 2.** $\mathbf{D}^{(k+1)} = \underset{\mathbf{D} \in \mathcal{S}}{\operatorname{argmin}} \|\mathbf{D} - (\mathbf{S} + \mathbf{U}_1)\|_F^2$
- Define $\mathcal{C}_1 = \{\mathbf{M} | \mathbf{M} = \mathbf{M}^\top, \operatorname{diag}(\mathbf{M}) = \mathbf{0}\}$ and $\mathcal{C}_2 = \{\mathbf{M} | \mathbf{M} \geq \mathbf{0}, \sum_{i=1}^N M_{1i} = 1\}$
 $\Rightarrow \mathcal{S} = \mathcal{C}_1 \cap \mathcal{C}_2$
 \Rightarrow Establish an inner ADMM for the \mathbf{D} -update [Boyd et al'11]

$$\begin{aligned} & \min_{\mathbf{E}, \mathbf{Z}} \quad \|\mathbf{E} - (\mathbf{S}^{(k+1)} + \mathbf{U}_1^{(k)})\|_F^2 + g_1(\mathbf{E}) + g_2(\mathbf{Z}) \\ & \text{s.to:} \quad \mathbf{E} - \mathbf{Z} = \mathbf{0}, \end{aligned}$$

- 1: **Input:** penalty parameter ρ_2 , number of iterations T_2 .
- 2: **Initialize:** $\mathbf{E}^{(0)} = \mathbf{Z}^{(0)} = \mathbf{U}_2^{(0)} = \mathbf{0}$.
- 3: **for** $i = 0, \dots, T_2 - 1$ **do**
- 4: $\mathbf{E}^{(i+1)} = \mathcal{P}_1\left(\frac{\mathbf{S}^{(k+1)} + \mathbf{U}_1^{(k)} + \frac{\rho_2}{2}(\mathbf{Z}^{(i)} - \mathbf{U}_2^{(i)})}{1 + \frac{\rho_2}{2}}\right) \Rightarrow \mathcal{P}_1(\mathbf{M}) = \frac{\mathbf{M} + \mathbf{M}^\top}{2} - \operatorname{Diag}(\mathbf{M})$
- 5: $\mathbf{Z}^{(i+1)} = \mathcal{P}_2(\mathbf{E}^{(i+1)} + \mathbf{U}_2^{(i)}) \Rightarrow$ Projection onto a simplex [Chen et al'11]
- 6: $\mathbf{U}_2^{(i+1)} = \mathbf{U}_2^{(i)} + \mathbf{E}^{(i+1)} - \mathbf{Z}^{(i+1)}$
- 7: **end for**
- 8: **return** $\mathbf{D}^{(k+1)} := \mathbf{E}^{(T_2)}$