

# Directed Network Topology Inference via Graph Filter Identification

Rasoul Shafipour, **Santiago Segarra**, Antonio G. Marques and Gonzalo Mateos

> Institute for Data, Systems, and Society Massachusetts Institute of Technology segarra@mit.edu http://www.mit.edu/~segarra/

Data Science Workshop, June 5, 2018

### Network Science analytics





### Desiderata: Process, analyze and learn from network data [Kolaczyk09]

### Network Science analytics





- Desiderata: Process, analyze and learn from network data [Kolaczyk09]
- ▶ Network as graph *G*: encode pairwise relationships
- Sometimes both G and data at the nodes are available ⇒ Leverage G to process network data ⇒ Graph Signal Processing

### Network Science analytics





- Desiderata: Process, analyze and learn from network data [Kolaczyk09]
- Network as graph G: encode pairwise relationships
- Sometimes both G and data at the nodes are available ⇒ Leverage G to process network data ⇒ Graph Signal Processing
- ► Sometimes we have access to network data but not to G itself
  ⇒ Leverage the relation between them to infer G from the data

# Graph signal processing: Notation



- ► Graph G with N nodes and adjacency A ⇒ A<sub>ii</sub> = Proximity between i and j
- ► Define a signal  $\mathbf{x} \in \mathbb{R}^N$  on top of the graph  $\Rightarrow x_i =$ Signal value at node i



# Graph signal processing: Notation



- ► Graph G with N nodes and adjacency A ⇒ A<sub>ii</sub> = Proximity between i and j
- ▶ Define a signal x ∈ ℝ<sup>N</sup> on top of the graph ⇒ x<sub>i</sub> = Signal value at node i



Associated with G is the graph-shift operator S = VAV<sup>-1</sup> ∈ ℝ<sup>N×N</sup>
 ⇒ S<sub>ij</sub> = 0 for i ≠ j and (i, j) ∉ E (local structure in G)
 ⇒ Ex: A and Laplacian L = D − A matrices



- ► Graph G with N nodes and adjacency A ⇒ A<sub>ii</sub> = Proximity between i and j
- ► Define a signal  $\mathbf{x} \in \mathbb{R}^N$  on top of the graph  $\Rightarrow x_i = \text{Signal value at node } i$



- Associated with G is the graph-shift operator S = VAV<sup>-1</sup> ∈ ℝ<sup>N×N</sup>
   ⇒ S<sub>ij</sub> = 0 for i ≠ j and (i, j) ∉ E (local structure in G)
   ⇒ Ex: A and Laplacian L = D − A matrices
- Graph filters  $\rightarrow$  Matrix polynomials:  $\mathbf{H} = \sum_{l=0}^{N-1} h_l \mathbf{S}^l = \mathbf{V} \operatorname{diag}(\tilde{\mathbf{h}}) \mathbf{V}^{-1}$
- Graph Signal Processing  $\rightarrow$  Exploit structure encoded in **S** to process **x**
- ► Take the reverse path. How to use GSP to infer the graph topology?

# Topology inference: Motivation and context

Network topology inference from nodal observations [Kolaczyk09]

- Partial correlations and conditional dependence [Dempster74]
- Sparsity [Friedman07] and consistency [Meinshausen06]
- [Banerjee08], [Lake10], [Slawski15], [Karanikolas16]
- Key in neuroscience [Sporns10]

 $\Rightarrow$  Functional net inferred from activity



# Topology inference: Motivation and context

Network topology inference from nodal observations [Kolaczyk09]

- Partial correlations and conditional dependence [Dempster74]
- Sparsity [Friedman07] and consistency [Meinshausen06]
- [Banerjee08], [Lake10], [Slawski15], [Karanikolas16]
- Key in neuroscience [Sporns10]
  - $\Rightarrow$  Functional net inferred from activity
- Noteworthy GSP-based approaches
  - Gaussian graphical models [Egilmez16]
  - Smooth signals [Dong15], [Kalofolias16]
  - Stationary signals [Pasdeloup15], [Segarra16]
  - Directed graphs [Mei15], [Shen16]
  - Low-rank excitation [Wai18]

### ► Contribution: Inference for directed networks from diffused signals





 $\blacktriangleright$  Signal **y** is the response of a linear network diffusion process to an input **x** 

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

 $\Rightarrow$  Structure of  $\boldsymbol{y}$  depends on structure of  $\boldsymbol{x}$  and  $\boldsymbol{S}$ 



 $\blacktriangleright$  Signal **y** is the response of a linear network diffusion process to an input **x** 

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

 $\Rightarrow$  Structure of  $\boldsymbol{y}$  depends on structure of  $\boldsymbol{x}$  and  $\boldsymbol{S}$ 

Cayley-Hamilton asserts we can write diffusion as

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

⇒ **y** is the output of a GF **H** ⇒ Use this and info on  $(\mathbf{y}, \mathbf{x})$  to find **S** ⇒ Key property: **H** is diagonalized by the eigenvectors of **S** 

• GF  $\equiv$  linear maps which are analytic functions of the sparse matrix **S** Ex.: **S**, **S**<sup>-1</sup>,  $(\mathbf{I} - \mathbf{S})^{-1}$ ,  $(\mathbf{I} - \alpha \mathbf{S})^{-2}$ ,  $(\mathbf{I} - \mathbf{S} - \mathbf{S}^2)^{-1}$ ,  $(\mathbf{I} - \beta \mathbf{S})(\mathbf{I} - \alpha \mathbf{S})^{-1}$ 



▶ We have access to *M* diffusion processes

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

► For each process, we gather the realizations  $\mathcal{Y}_m := \{\mathbf{y}_m^{(p)}\}_{p=1}^{P_m}$ 

⇒ Every realization corresponds to an independent input  $\mathbf{x}_m^{(p)}$ ► We do not have access to *L*, *h*<sub>l</sub>, or the inputs

 $\Rightarrow$  We do know that inputs are zero mean with covariance  $C_{x,m}$ 



We have access to M diffusion processes

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

▶ For each process, we gather the realizations  $\mathcal{Y}_m := \{\mathbf{y}_m^{(p)}\}_{p=1}^{P_m}$ 

⇒ Every realization corresponds to an independent input  $\mathbf{x}_m^{(p)}$ ► We do not have access to *L*, *h*<sub>l</sub>, or the inputs

 $\Rightarrow$  We do know that inputs are zero mean with covariance  $C_{x,m}$ 

**Problem**: Given observations  $\mathcal{Y} = \bigcup_{m=1}^{M} \mathcal{Y}_m$  and the input covariances  $C_{x,m}$ , find sparsest (asymmetric) **S** that is consistent with the observations









The covariance matrix of the output process y<sub>m</sub> is

$$\mathbf{C}_{\mathbf{y},m} = \mathbb{E}\left[\mathbf{H}\mathbf{x}_m (\mathbf{H}\mathbf{x}_m)^T\right] = \mathbf{H}\mathbb{E}\left[\mathbf{x}_m \mathbf{x}_m^T\right]\mathbf{H}^T = \mathbf{H}\mathbf{C}_{\mathbf{x},m}\mathbf{H}^T$$

► Each obs. pair C<sub>y,m</sub> = HC<sub>x,m</sub>H<sup>T</sup> gives rise to a set of potential solutions ⇒ Intersection smaller (unique) as M ↑, try to solve





The covariance matrix of the output process y<sub>m</sub> is

$$\mathbf{C}_{\mathbf{y},m} = \mathbb{E}\left[\mathbf{H}\mathbf{x}_m (\mathbf{H}\mathbf{x}_m)^T\right] = \mathbf{H}\mathbb{E}\left[\mathbf{x}_m \mathbf{x}_m^T\right] \mathbf{H}^T = \mathbf{H}\mathbf{C}_{\mathbf{x},m} \mathbf{H}^T$$

► Each obs. pair  $\mathbf{C}_{\mathbf{y},m} = \mathbf{H}\mathbf{C}_{\mathbf{x},m}\mathbf{H}^T$  gives rise to a set of potential solutions  $\Rightarrow$  Intersection smaller (unique) as  $M \uparrow$ , try to solve  $\underset{\mathbf{H}_{\mathsf{L}},\mathbf{H}_{\mathsf{R}}\in\mathcal{M}_N}{\operatorname{argmin}} \sum_{m=1}^{M} ||\mathbf{C}_{\mathbf{y},m} - \mathbf{H}_{\mathsf{L}}\mathbf{C}_{\mathbf{x},m}\mathbf{H}_{\mathsf{R}}^T||_F^2$  s. to  $\mathbf{H}_{\mathsf{L}} = \mathbf{H}_{\mathsf{R}}$ 

 $\Rightarrow$  Variables of size  $N^2$ , smarter way to formulate the recovery?  $\Rightarrow$  Parametrize the set of feasible solutions



▶ For each *m*, we have a matrix equation of the form

$$\mathbf{C}_{\mathbf{y},m} = \mathbf{H}\mathbf{C}_{\mathbf{x},m}\mathbf{H}^{T} \tag{1}$$



▶ For each *m*, we have a matrix equation of the form

$$\mathbf{C}_{\mathbf{y},m} = \mathbf{H}\mathbf{C}_{\mathbf{x},m}\mathbf{H}^{T} \tag{1}$$

If  $C_{x,m}$  and  $C_{y,m}$  are full rank, the set  $\mathcal{H}_m$  containing all the (possibly asymmetric) matrices **H** that solve (1) for a particular *m* is given by

$$\mathcal{H}_m = \{ \mathbf{H} \mid \mathbf{H} = \mathbf{C}_{\mathbf{y},m}^{1/2} \mathbf{U} \mathbf{C}_{\mathbf{x},m}^{-1/2} \text{ and } \mathbf{U} \mathbf{U}^T = \mathbf{I} \}.$$

141iT

▶ For each *m*, we have a matrix equation of the form

$$\mathbf{C}_{\mathbf{y},m} = \mathbf{H}\mathbf{C}_{\mathbf{x},m}\mathbf{H}^{T}$$
(1)

If  $C_{x,m}$  and  $C_{y,m}$  are full rank, the set  $\mathcal{H}_m$  containing all the (possibly asymmetric) matrices **H** that solve (1) for a particular *m* is given by

$$\mathcal{H}_m = \{ \mathbf{H} \mid \mathbf{H} = \mathbf{C}_{\mathbf{y},m}^{1/2} \mathbf{U} \mathbf{C}_{\mathbf{x},m}^{-1/2} \text{ and } \mathbf{U} \mathbf{U}^T = \mathbf{I} \}.$$

Optimization over unitary matrices

 $\Rightarrow N(N-1)/2$  degrees of freedom in lieu of  $N^2$ 

 $\Rightarrow$  Each *m* kills N(N+1)/2 degrees of freedom  $\Rightarrow M = 2$  may suffice

 $\Rightarrow$  Non convex, but tailored algorithms are available

▶ Solving system id (non-symm. square roots) by leveraging structure

# Manopt for non-symmetric graph-filter id

Original formulation:

$$\underset{\mathsf{H}_{\mathsf{L}},\mathsf{H}_{\mathsf{R}}}{\operatorname{argmin}} \sum_{m=1}^{M} || \hat{\mathsf{C}}_{\mathsf{y},m} - \mathsf{H}_{\mathsf{L}} \mathsf{C}_{\mathsf{x},m} \mathsf{H}_{\mathsf{R}}^{\mathsf{T}} ||_{F}^{2} \quad \text{s. to } \mathsf{H}_{\mathsf{L}} = \mathsf{H}_{\mathsf{R}} \quad (\mathcal{P}1)$$

- ► Leveraging structure: optimize over  $\mathbf{U}_m \in \mathcal{U}_N$   $\underset{\mathbf{H}, \{\mathbf{U}_m\}_{m=1}^M}{\operatorname{argmin}} \sum_{m=1}^M \|\mathbf{H} - \hat{\mathbf{C}}_{\mathbf{y},m} \mathbf{U}_m \mathbf{C}_{\mathbf{x},m}^{-1/2}\|_F^2 \quad (\mathcal{P}2)$ 
  - ⇒ Approach: projected gradient descent (manopt)
  - $\Rightarrow$  Sensitive to initialization

# Manopt for non-symmetric graph-filter id

Original formulation:

$$\underset{\mathsf{H}_{\mathsf{L}},\mathsf{H}_{\mathsf{R}}}{\operatorname{argmin}} \sum_{m=1}^{M} || \hat{\mathsf{C}}_{\mathsf{y},m} - \mathsf{H}_{\mathsf{L}} \mathsf{C}_{\mathsf{x},m} \mathsf{H}_{\mathsf{R}}^{\mathsf{T}} ||_{\mathsf{F}}^{2} \quad \text{s. to } \mathsf{H}_{\mathsf{L}} = \mathsf{H}_{\mathsf{R}} \quad (\mathcal{P}1)$$

- ► Leveraging structure: optimize over  $\mathbf{U}_m \in \mathcal{U}_N$   $\underset{\mathbf{H}, \{\mathbf{U}_m\}_{m=1}^M}{\operatorname{argmin}} \sum_{m=1}^M \|\mathbf{H} - \hat{\mathbf{C}}_{\mathbf{y},m} \mathbf{U}_m \mathbf{C}_{\mathbf{x},m}^{-1/2}\|_F^2 \quad (\mathcal{P}2)$ 
  - ⇒ Approach: projected gradient descent (manopt)
  - $\Rightarrow$  Sensitive to initialization

Enhanced algorithm: Smart initialization + Projected gradient

(s1) Use ( $\mathcal{P}$ 1) to find  $\hat{\mathbf{H}}_{L}^{(0)}$  initial estimate of  $\mathbf{H}$ 

(s2) Use the  $\hat{\mathbf{H}}_{L}^{(0)}$  generated by (s1) as input for ( $\mathcal{P}$ 2) to obtain  $\hat{\mathbf{H}}$ 





# GSO inference



- Finding **S** from  $\mathbf{H} = h_0 \mathbf{I} + h_1 \mathbf{S} + h_2 \mathbf{S}^2$  non-convex but...
  - $\Rightarrow$  S and H are simultaneously diagonalizable

# GSO inference



Finding **S** from  $\mathbf{H} = h_0 \mathbf{I} + h_1 \mathbf{S} + h_2 \mathbf{S}^2$  non-convex but...

 $\Rightarrow$  S and H are simultaneously diagonalizable

► We can use extra knowledge/assumptions to choose one graph ⇒ Of all graphs, select one that sparsest one

► Set *S* contains all admissible scaled adjacency matrices

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

# GSO inference



Finding **S** from  $\mathbf{H} = h_0 \mathbf{I} + h_1 \mathbf{S} + h_2 \mathbf{S}^2$  non-convex but...

 $\Rightarrow$  S and H are simultaneously diagonalizable

► We can use extra knowledge/assumptions to choose one graph ⇒ Of all graphs, select one that sparsest one

► Set *S* contains all admissible scaled adjacency matrices

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

In practice we solve the robust convex relaxation

$$\begin{split} \mathbf{S}^* &:= \underset{\mathbf{S}}{\operatorname{argmin}} \ \|\mathbf{S}\|_1 \quad \text{ s. to } \ \|\hat{\mathbf{H}}\mathbf{S}-\mathbf{S}\hat{\mathbf{H}}\|_{\mathrm{F}} \leq \epsilon, \ \mathbf{S} \in \mathcal{S} \end{aligned}$$



- Consider Erdős-Rényi digraphs with 20 nodes and link probability p
  - $\Rightarrow$  Generate covariances as  $\mathbf{C}_{\mathbf{x},m} = \mathbf{B}_m \mathbf{B}_m^T$ , with  $\mathbf{B}_m$  normal
  - $\Rightarrow$  Diffusing filters: FIR with L = 3



- Recovery for different M and p averaged for 10 graphs
  - $\Rightarrow$  Recovery increases with M
  - $\Rightarrow$  For high *p* fails oftentimes due to sparse recovery (Step 2)

|||iT

Social net. G of N = 32 students in a class at the University of Ljubljana
 Directed edges between students represent perceived friendships
 Signals generated synthetically: FIR and IIR



Recov. over 10 realizations as a function of M and P = 10<sup>6</sup> (left)
 M = 5, P = 10<sup>4</sup> filtered by FIR (right)

Conclusions



Conclusions



- Guarantees for system ID (manifold optimization)
- Guarantees for GSO inference
- Incorporation of priors on the filter and the GSO



### Symposium on Graph Signal Processing

#### Topics of interest

- $\cdot$  Graph-signal transforms and filters
- $\cdot$  Distributed and non-linear graph SP
- · Statistical graph SP
- · Prediction and learning for graphs
- · Network topology inference
- · Recovery of sampled graph signals
- · Control of network processes

#### Paper submission due: June 17, 2018



- $\cdot$  Signals in high-order and multiplex graphs
- $\cdot$  Neural networks for graph data
- · Topological data analysis
- $\cdot$  Graph-based image and video processing
- $\cdot$  Communications, sensor and power networks
- · Neuroscience and other medical fields
- $\cdot$  Web, economic and social networks

#### Organizers:

Gonzalo Mateos (Univ. of Rochester)

Santiago Segarra (MIT)

Sundeep Chepuri (TU Delft)