

Identifying Undirected Network Structure via Semidefinite Relaxation

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/

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Network Science analytics





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

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- ▶ 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

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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 (GSP)



- ► Undirected G with adjacency matrix A ⇒ A_{ij} = Proximity between i and j
- ▶ Define a signal x on top of the graph ⇒ x_i = Signal value at node i



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Associated with G is the graph-shift operator S = VAV^T ∈ M^N
 ⇒ S_{ij} = 0 for i ≠ j and (i, j) ∉ E (local structure in G)
 ⇒ Ex: adjacency A and Laplacian L = D − A matrices

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- ► Associated with G is the graph-shift operator $\mathbf{S} = \mathbf{V} \mathbf{\Lambda} \mathbf{V}^T \in \mathcal{M}^N$
 - \Rightarrow $S_{ij} = 0$ for $i \neq j$ and $(i, j) \notin \mathcal{E}$ (local structure in G)
 - \Rightarrow Ex: adjacency **A** and Laplacian **L** = **D A** matrices
- Graph filters H : ℝ^N → ℝ^N are maps between graph signals
 ⇒ Polynomial in S with coefficients h ∈ ℝ^{L+1} ⇒ H := ∑^L_{l=0} h_lS^l
- 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



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- 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]
- ▶ Our contribution: topology inference from non-stationary graph signals



Problem formulation



- Underlying graph \mathcal{G} with undirected unknown GSO **S**
- Observe signals $\{\mathbf{y}_i\}_{i=1}^K$ defined on the unknown graph





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Problem statement

Given observations $\{\mathbf{y}_i\}_{i=1}^{K}$, determine the network **S** knowing that: $\{\mathbf{y}_i\}_{i=1}^{K}$ are outputs of a diffusion process on **S**.

5/18



► Consider an arbitrary linear network process on the GSO S ⇒ Every realization corresponds to a different input x_i

$$\mathbf{y}_i = \left(\sum_{l=0}^{L} h_l \mathbf{S}^l\right) \mathbf{x}_i = \mathbf{H} \mathbf{x}_i, \quad i = 1, \dots, K$$

- **Goal**: Recover **S** from the observation of K signals $\{\mathbf{y}_i\}_{i=1}^{K}$
- Additional unknowns
 - \Rightarrow The degree of the filter L
 - \Rightarrow The filter coefficients $\{h_l\}_{l=0}^{L}$
 - \Rightarrow The specific inputs \mathbf{x}_i ; but we know that $\mathbf{x}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{C}_{\mathbf{x}})$

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▶ y is the output of a local diffusion process on the graph

$$\mathbf{y} = \alpha_0 \prod_{l=1}^{\infty} (\mathbf{I} - \alpha_l \mathbf{S}) \mathbf{x} = \left(\sum_{l=0}^{N-1} h_l \mathbf{S}^l \right) \mathbf{x} := \mathbf{H} \mathbf{x}$$

Whenever the input x is white

 \Rightarrow graph stationary process on **S** [Marques17, Girault15, Perraudin17]

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Stationary case

► The covariance C_y of y shares V with S

$$C_y = H^2 = h_0^2 I + 2h_0 h_1 S + h_1^2 S^2 + \dots$$

• Estimate covariance from $\{\mathbf{y}_i\}_{i=1}^K$ as $\hat{\mathbf{C}}_{\mathbf{y}} \Rightarrow \text{Diagonalize} \Rightarrow \text{Obtain } \hat{\mathbf{V}}$

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- ▶ Q: What if the signal y = Hx is not stationary (i.e., x colored)?
 - \Rightarrow Matrices S and C_y no longer simultaneously diagonalizable since

$$C_y = HC_xH$$

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► Q: What if the signal y = Hx is not stationary (i.e., x colored)?
⇒ Matrices S and Cy no longer simultaneously diagonalizable since

$\mathbf{C}_{\mathbf{y}} = \mathbf{H}\mathbf{C}_{\mathbf{x}}\mathbf{H}$

Key: still H = ∑_{l=0}^{L-1} h_lS^l diagonalized by the eigenvectors V of S
 ⇒ Infer V by estimating the unknown diffusion (graph) filter H
 ⇒ Step 1 boils down to system identification + eigendecomposition

$$\{\mathbf{y}_i\}_{i=1}^K \longrightarrow \begin{array}{c} \text{System} & \hat{\mathbf{H}} \\ \text{Identification} & & & & & \\ \end{array}$$
 Eigendecomposition $\rightarrow \hat{\mathbf{V}}$



Define $C_{xyx} := C_x^{1/2}C_yC_x^{1/2}$, with eigenvectors V_{xyx} . If C_x is non-singular then all admissible symmetric filters H are of the form

 $\mathbf{H} = \mathbf{C}_{\mathbf{x}}^{-1/2} \mathbf{C}_{\mathbf{x}\mathbf{y}\mathbf{x}}^{1/2} \mathbf{V}_{\mathbf{x}\mathbf{y}\mathbf{x}} \mathsf{diag}(\mathbf{b}) \mathbf{V}_{\mathbf{x}\mathbf{y}\mathbf{x}}^{T} \mathbf{C}_{\mathbf{x}}^{-1/2},$

where $\mathbf{b} \in \{-1, 1\}^N$ is a binary (signed) vector.

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where $\mathbf{b} \in \{-1, 1\}^N$ is a binary (signed) vector.

- Even if we get C_y exactly, H is not identifiable
 - \Rightarrow Not surprising since we only have second moment info
- ► Consider having access to multiple input distributions {C_{x,m}}^M_{m=1}

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Multiple input processes



► Define
$$\mathbf{A}_m := (\mathbf{C}_{\mathbf{x},m}^{-1/2} \mathbf{V}_{\mathbf{xyx},m}) \odot (\mathbf{C}_{\mathbf{x},m}^{-1/2} \mathbf{C}_{\mathbf{xyx},m}^{1/2} \mathbf{V}_{\mathbf{xyx},m})$$

 $\Psi := \begin{bmatrix} \mathbf{A}_1 & -\mathbf{A}_2 & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_2 & -\mathbf{A}_3 & \cdots & \mathbf{0} & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{A}_{M-1} & -\mathbf{A}_M \end{bmatrix}$
 $\mathbf{b}_m \in \{-1,1\}^N \text{ and } \mathbf{b} = [\mathbf{b}_1^T, \mathbf{b}_2^T, \dots, \mathbf{b}_M^T]^T, \text{ then } \Psi \mathbf{b}^* = \mathbf{0}$

11/18

Santiago Segarra

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$$\mathbf{b}_m \in \{-1,1\}^N \text{ and } \mathbf{b} = [\mathbf{b}_1^T, \mathbf{b}_2^T, \dots, \mathbf{b}_M^T]^T, \text{ then } \Psi \mathbf{b}^* = \mathbf{0}$$
Whenever only estimates $\hat{\mathbf{C}}_{\mathbf{y},m}$ are available, we can estimate \mathbf{b}^* as

$$\hat{\mathbf{b}}^* = \underset{\mathbf{b} \in \{-1,1\}^{\textit{NM}}}{\operatorname{argmin}} \mathbf{b}^T \hat{\boldsymbol{\Psi}}^T \hat{\boldsymbol{\Psi}} \mathbf{b},$$

obtaining our estimate for the filter ${\bf H}$ as

$$\hat{\mathbf{H}} = \frac{1}{M} \sum_{m=1}^{M} \mathbf{C}_{\mathbf{x},m}^{-1/2} \hat{\mathbf{C}}_{\mathbf{x}\mathbf{y}\mathbf{x},m}^{1/2} \hat{\mathbf{V}}_{\mathbf{x}\mathbf{y}\mathbf{x},m} \text{diag}(\hat{\mathbf{b}}_{m}^{*}) \hat{\mathbf{V}}_{\mathbf{x}\mathbf{y}\mathbf{x},m}^{T} \mathbf{C}_{\mathbf{x},m}^{-1/2}$$

Our problem then reduces to solving the BQP

$$\hat{\mathbf{b}}^* = \operatorname*{argmin}_{\mathbf{b} \in \{-1,1\}^{NM}} \mathbf{b}^T \hat{\mathbf{\Psi}}^T \hat{\mathbf{\Psi}} \mathbf{b}$$

► Define
$$\hat{\mathbf{W}} = \hat{\mathbf{\Psi}}^T \hat{\mathbf{\Psi}}$$
 and $\mathbf{B} = \mathbf{b}\mathbf{b}^T$
min tr $(\hat{\mathbf{W}}\mathbf{B})$ s. to rank $(\mathbf{B}) = 1, \ B_{ii} = 1, \ i = 1, \dots, NM$

Drop source of non-convexity to obtain the semi-definite relaxation

$$\mathbf{B}^* = \operatorname*{argmin}_{\mathbf{B} \succeq \mathbf{0}} \operatorname{tr}(\hat{\mathbf{W}}\mathbf{B}) \quad \text{s. to } \quad B_{ii} = 1, \ i = 1, \dots, NM$$

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► For l = 1, ..., L, draw $\mathbf{z}_l \sim \mathcal{N}(\mathbf{0}, \mathbf{B}^*)$, round $\tilde{\mathbf{b}}_l = \operatorname{sign}(\mathbf{z}_l)$, to obtain $l^* = \underset{l=1,...,L}{\operatorname{argmin}} \tilde{\mathbf{b}}_l^T \hat{\mathbf{W}} \tilde{\mathbf{b}}_l$



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Let \hat{b}^* be the true solution of the BQP and let \tilde{b}_{\prime^*} be the output of our method. Then,

$$(\hat{\mathbf{b}}^*)^T \hat{\mathbf{W}} \hat{\mathbf{b}}^* \leq \mathbb{E}\left[(\tilde{\mathbf{b}}_{l^*})^T \hat{\mathbf{W}} \tilde{\mathbf{b}}_{l^*} \right] \leq \frac{2}{\pi} (\hat{\mathbf{b}}^*)^T \hat{\mathbf{W}} \hat{\mathbf{b}}^* + \gamma,$$

where $\gamma = \left(1 - \frac{2}{\pi}\right) \lambda_{\max} NM$.

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► We can use extra knowledge/assumptions to choose one graph

 \Rightarrow Of all graphs, select one that is optimal in some sense

$$\hat{\mathbf{S}} := \operatorname*{argmin}_{\mathbf{S}, \boldsymbol{\lambda}} f(\mathbf{S}, \boldsymbol{\lambda})$$
 s. to $\mathbf{S} = \sum_{k=1}^{N} \lambda_k \mathbf{v}_k \mathbf{v}_k^T$, $\mathbf{S} \in S$

▶ Set *S* contains all admissible scaled adjacency matrices

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

 \Rightarrow Can accommodate Laplacian matrices as well

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- Problem is convex if we select a convex objective f(S, λ)
 Ex: Sparsity (f(S) = ||S||₁), min. energy (f(S) = ||S||_F), mixing (f(λ) = −λ₂)
- Robust recovery from imperfect or incomplete V [Segarra16]

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Unveiling urban mobility patterns



- Detect mobility patterns in New York City from Uber pickup data
- Times and locations (N = 30) from January 1st to June 29th 2015
- M = 2 graph processes: weekday (m = 1) and weekend (m = 2) pickups
- Pickups within 6-11am as input signal x and 3-8pm as output y







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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)

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Santiago Segarra (MIT)

Sundeep Chepuri (TU Delft)