Robust Graph Filter Identification and Graph Denoising from Signal Observations

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Graph Signal Processing Workshop 2023 (GSP 2023) - Oxford, United Kingdom - June 12-14, 2023

Why a robust GSP framework?

- Data is becoming heterogeneous and pervasive [Kolaczyk09][Leskovec20]
  - Often defined over irregular domains and networks
  - More complex structure demands more complex architectures
- **GSP**: models data structure as a graph [Shuman13][Ortega18]
  - Leverages the graph topology to process the data

Social network

Brain network

Home automation network

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- **GSP**: models data structure as a graph [Shuman13][Ortega18]
  - Leverages the graph topology to process the data
- **Problem:** data is prone to errors and imperfections
  - Noise, missing values, or outliers are pervasive in data science

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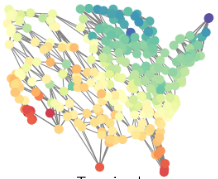
- Signal processing deals with perturbations on the signals
  - Large perturbations render data useless
  - Widely study in several fields



True signal

Noisy signal

- Signal processing deals with perturbations on the signals
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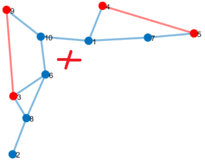
- In GSP we encounter perturbations in the graph topology
  - Even small perturbations lead to challenging problems
  - Most GSP methods assume the graph is perfectly known

Original graph



Errors in the support

Noisy edges

Imperfections in the graph topology

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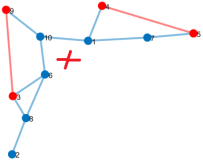

Errors in the support

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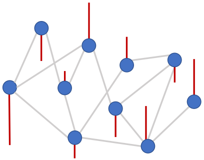
- **This work**: approach the graph FI accounting for topology imperfections

Fundamentals of GSP

- Graph $G = (V, E)$ with N nodes and adjacency $\mathbf{A}$
  - A_{ij} = Proximity between i and j



- Define a signal $\mathbf{x} \in \mathbb{R}^N$ on top of the graph
  - x_i = Signal value at node i
- Associated with G is the graph-shift operator $\mathbf{S} \in \mathbb{R}^{N \times N}$ (e.g. $\mathbf{A}$, $\mathbf{L}$)
  - $S_{ij} \neq 0$ if $i = j$ or $(i, j) \in E$ (local structure in G) [Shuman13][Sandryhaila13]
  - Diagonalized as $\mathbf{S} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}$

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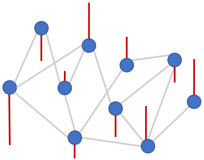

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- Graph filters are defined as $\mathbf{H} = \sum_{r=0}^{R-1} h_r \mathbf{S}^r$ [Segarra17]
    - Diagonalized as $\mathbf{H} = \mathbf{V}\text{diag}(\tilde{\mathbf{h}})\mathbf{V}^{-1}$
    - $\mathbf{S}^r$ encodes r-hop neighborhood so $\mathbf{H}\mathbf{x}$ diffuses $\mathbf{x}$ across G

GF ID and influence of perturbations

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- **GF identification:** estimate the graph filter $\mathbf{H} = \sum_{r=0}^{R-1} h_r \mathbf{S}^r$
  - Given input/output signals $\mathbf{X}/\mathbf{Y} \in \mathbb{R}^{N \times M}$ with $\mathbf{Y} = \mathbf{H}\mathbf{X} + \mathbf{W}$
  - Leveraging that $\mathbf{H}$ is a polynomial of the GSO

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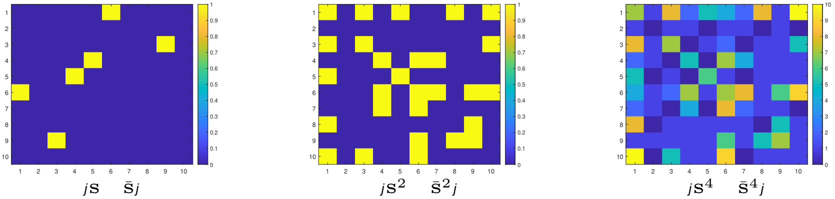
- Due to perturbations the true $\mathbf{S}$ is **unknown**
  - → Only perturbed $\bar{\mathbf{S}} \in \mathbb{R}^{N \times N}$ is observed
- **Q:** What if we estimate the filter as $\mathbf{H} = \sum_{r=0}^{R-1} h_r \bar{\mathbf{S}}^r$?
  - → Error between $\mathbf{S}^r$ and $\bar{\mathbf{S}}^r$ grows with r



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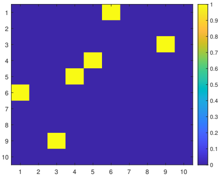
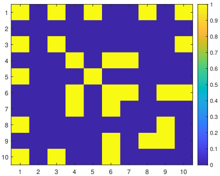
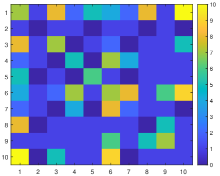
- **A:** estimating $\mathbf{H}$ as polynomial of $\bar{\mathbf{S}}$ results in **high estimation error**



$|\mathbf{S} - \bar{\mathbf{S}}|$



$|\mathbf{S}^2 - \bar{\mathbf{S}}^2|$



$|\mathbf{S}^4 - \bar{\mathbf{S}}^4|$

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Modeling graph perturbations

- Additive perturbation models are pervasive in SP $\Rightarrow$ In graphs $\bar{\mathbf{S}} = \mathbf{S} + \mathbf{\Delta}$
  - $\Rightarrow$ Structure of $\mathbf{\Delta} \in \mathbb{R}^{N \times N}$ depends on the type of perturbation
  - $\Rightarrow$ $\mathbf{S}$ and $\bar{\mathbf{S}}$ are close according to some metric $d(\mathbf{S}, \bar{\mathbf{S}})$

Graph perturbations

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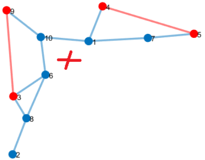
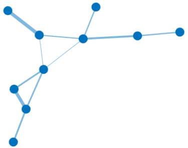
Examples of topology perturbations

- When perturbations **create/destroy edges** $\Longrightarrow$ $d(\mathbf{S}, \bar{\mathbf{S}}) = \|\mathbf{S} - \bar{\mathbf{S}}\|_0$
  - $\Rightarrow$ $\Delta_{ij} = 1$ if $S_{ij} = 0$ and $\Delta_{ij} = -1$ if $S_{ij} = 1$
- When perturbations represent **noisy edges** $\Longrightarrow$ $d(\mathbf{S}, \bar{\mathbf{S}}) = \|\mathbf{S}_E - \bar{\mathbf{S}}_E\|_2^2$
  - $\Rightarrow$ $\Delta_{ij} = 0$ if $S_{ij} = 0$ and $\Delta_{ij} \sim \mathcal{N}(0, \sigma^2)$ if $S_{ij} \neq 0$


Original graph



Create/Destroy edges


Noisy edges

Traditional filter identification (FI)

- Consider formulation in either vertex or frequency domain

$$\min_{\mathbf{h}} \|\mathbf{Y} - \sum_{k=0}^{N-1} h_k \mathbf{S}^k \mathbf{X}\|_F^2 \qquad \min_{\tilde{\mathbf{h}}} \|\mathbf{Y} - \mathbf{V}\text{diag}(\tilde{\mathbf{h}})\mathbf{V}^\top \mathbf{X}\|_F^2$$

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$$\text{s. t.} \quad \mathbf{S} \in \mathcal{S} \qquad\qquad \text{s. t.} \quad \mathbf{V}\mathbf{V}^\top = \mathbf{I}$$

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Robust filter identification (RFI)

- Define full $\mathbf{H}$ as an optimization variable and jointly estimate $\mathbf{H}$ and $\mathbf{S}$

$$\min_{\mathbf{S}\in\mathcal{S},\mathbf{H}} \|\mathbf{Y} - \mathbf{H}\mathbf{X}\|_F^2 + \lambda d(\mathbf{S},\bar{\mathbf{S}}) + \beta\|\mathbf{S}\|_0 \quad \text{s. t. } \mathbf{S}\mathbf{H} = \mathbf{H}\mathbf{S}$$

  - ⇒ The constraint captures the fact that $\mathbf{H}$ is a polynomial of $\mathbf{S}$
  - ⇒ Second term promotes closeness between $\bar{\mathbf{S}}$ and $\mathbf{S}$

- Operates in vertex domains + avoids computation of high-order polynomials
- Bilinear terms and ℓ_0 render the problem non-convex

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Dealing with ℓ_0 norm

- We employ the ℓ_1 reweighted norm based on logarithmic penalty [Candes08]

$$\|\mathbf{Z}\|_0 \quad r_\delta(\mathbf{Z}) := \sum_{i=1}^{I} \sum_{j=1}^{J} \log(|Z_{ij}| + \delta)$$

  - Produces sparser solutions than ℓ_1 norm
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Dealing with bilinear term

- Adopt an alternating-minimization approach to break the non-linearity
  - $\mathbf{H}$ and $\mathbf{S}$ are estimated in two separate iterative steps
  - Each step requires solving a convex optimization problem

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- Rewrite optimization problem as

$$\min_{\mathbf{S}\in\mathcal{S},\mathbf{H}} \|\mathbf{Y}-\mathbf{H}\mathbf{X}\|_F^2+\lambda r_{\delta_1}(\mathbf{S}-\bar{\mathbf{S}})+\beta r_{\delta_2}(\mathbf{S})+\gamma\|\mathbf{S}\mathbf{H}-\mathbf{H}\mathbf{S}\|_F^2$$

  - Constraint $\mathbf{S}\mathbf{H}=\mathbf{H}\mathbf{S}$ relaxed as a regularizer

- **Step 1 - GF Identification**: estimate $\mathbf{H}^{(t+1)}$ with $\mathbf{S}^{(t)}$ fixed

$$\mathbf{H}^{(t+1)} = \arg\min_{\mathbf{H}} \|\mathbf{Y} - \mathbf{H}\mathbf{X}\|_F^2 + \gamma \|\mathbf{S}^{(t)}\mathbf{H} - \mathbf{H}\mathbf{S}^{(t)}\|_F^2$$

  - LS problem with closed-form solution inverting an $N^2 \times N^2$ matrix

- **Step 2 - Graph Denoising**: estimate $\mathbf{S}^{(t+1)}$ with $\mathbf{H}^{(t+1)}$ fixed

$$\mathbf{S}^{(t+1)} = \arg\min_{\mathbf{S} \in \mathcal{S}} \sum_{i,j=1}^{N} \left(\lambda \; {}_{ij}^{(t)} |S_{ij} - \bar{S}_{ij}| + \beta \; {}_{ij}^{(t)} |S_{ij}|\right) + \gamma \|\mathbf{S}\mathbf{H}^{(t+1)} - \mathbf{H}^{(t+1)}\mathbf{S}\|_F^2$$

  - With ℓ_1 weights ${}_{ij}^{(t)}$, ${}_{ij}^{(t)}$ computed from previous GSO $\mathbf{S}^{(t)}$

- Steps 1 and 2 repeated for $t = 0, ..., t_{max} - 1$ iterations

Alternating optimization algorithm

- **Step 1 - GF Identification**: estimate $\mathbf{H}^{(t+1)}$ with $\mathbf{S}^{(t)}$ fixed

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Theorem

The RFI algorithm **converges to an stationary** point if $\mathbf{S}$ does not have repeated eigenvalues and every row of $\tilde{\mathbf{X}} = \mathbf{V}^{-1}\mathbf{X}$ are nonzero

- Now the goal is to estimate K GFs $\{\mathbf{H}_k\}_{k=1}^{K}$
  - For each $\mathbf{H}_k$ we have M_k input/output signals $\mathbf{X}_k/\mathbf{Y}_k$
- Several GFs show up in relevant settings [Segarra16][Isufi16]
  - Different network processes on a graph $\mathbf{Y}_k = \mathbf{H}_k\mathbf{X}_k + \mathbf{W}_k$
  - Graph-based multivariate time series $\mathbf{Y}_\kappa = \sum_{k=1}^{K}\mathbf{H}_k\mathbf{Y}_{\kappa-k} + \mathbf{X}_\kappa + \mathbf{W}_k$

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  - Graph-based multivariate time series $\mathbf{Y}_\kappa = \sum_{k=1}^{K}\mathbf{H}_k\mathbf{Y}_{\kappa-k} + \mathbf{X}_\kappa + \mathbf{W}_k$
- Joint identification exploits each $\mathbf{H}_k$ being a polynomial on $\mathbf{S}$

$$\min_{\mathbf{S}\in\mathcal{S},\{\mathbf{H}_k\}_{k=1}^{K}} \sum_{k=1}^{K}\alpha_k\|\mathbf{Y}_k-\mathbf{H}_k\mathbf{X}_k\|_F^2+\lambda r_{\delta_1}(\mathbf{S}-\bar{\mathbf{S}})+\beta r_{\delta_2}(\mathbf{S})+\sum_{k=1}^{K}\gamma\|\mathbf{S}\mathbf{H}_k-\mathbf{H}_k\mathbf{S}\|_F^2$$

  - K commutativity constraints improve estimation of $\mathbf{S}$
  - A better estimate of $\mathbf{S}$ leads to better estimates of $\mathbf{H}_k$
- Solved via 2-step alternating optimization

Efficient implementation

- RFI algorithm has a computational complexity of $O(N^7)$
  - Prohibitive for large graphs
  - Steps 1 and 2 can be accelerated via an iterative process

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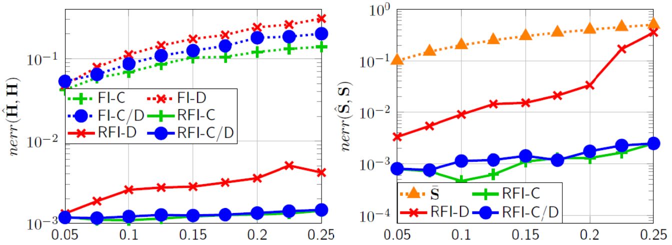
- RFI algorithm has a computational complexity of $O(N^7)$
  - Prohibitive for large graphs
  - Steps 1 and 2 can be accelerated via an iterative process
- **Step 1 - Efficient GF Identification**
  - Estimate $\mathbf{H}^{(t+1)}$ performing τ_{max_1} iterations of gradient descent
  - Involves multiplications of $N \times N$ matrices
- **Step 2 - Efficient Graph Denoising**
  - Estimate $\mathbf{S}^{(t+1)}$ via alternating optimization for τ_{max_2}
  - Solve N^2 scalar problems
  - Closed-form solution based on projected soft-thresholding
- Computational complexity reduced to $O(N^3)$

Numerical Evaluation (I)

- Test the estimates $\hat{\mathbf{H}}$ and $\hat{\mathbf{S}}$ with and without robust approach
  - Graphs are sampled from the small-world random graph model
  - We consider different types of perturbations



(a) Proportion of perturbed links (b) Proportion of perturbed links

- RFI consistently outperforms classical FI
  - Clear improvement in estimation of $\mathbf{S}$ with respect to $\bar{\mathbf{S}}$
- Only destroying links is the most damaging perturbation

Numerical Evaluation (II)

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- **Dataset**: 5-nearest neighbor graph of weather stations in California
  - Signals are temperature measurements
- **Goal:** Predict temperature 1 or 3 days in the future
  - Estimate $\mathbf{H}$ using 25% or 50% of the available data
- Consider LS as a naive solution and TLS-SEM as a robust baseline

Models	1-Step		3-Step	
	TTS=0.25	TTS = 0.5	TTS=0.25	TTS = 0.5
LS	$6.9 \; 10^{\;3}$	$3.1 \; 10^{\;3}$	$2.1 \; 10^{\;2}$	$9.1 \; 10^{\;3}$
LS-GF	$3.3 \; 10^{\;3}$	$3.3 \; 10^{\;3}$	$8.4 \; 10^{\;3}$	$8.5 \; 10^{\;3}$
TLS-SEM	$4.0 \; 10^{1}$	$3.7 \; 10^{\;2}$	$6.8 \; 10^{\;1}$	$5.5 \; 10^{\;2}$
RFI	$3.4 \; 10^{\;3}$	$3.1 \; 10^{\;3}$	$8.5 \; 10^{\;3}$	$7.5 \; 10^{\;3}$
AR(3)-RFI	$\mathbf{3.2 \; 10^{\;3}}$	$\mathbf{2.8 \; 10^{\;3}}$	$\mathbf{7.8 \; 10^{\;3}}$	$\mathbf{6.9 \; 10^{\;3}}$

- Best performance achieved by joint inference assuming AR model of order 3
  - Follow up closely by the (separate) RFI algorithm

Closing remarks

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- Proposed a general robust graph filter identification model that
  - Simultaneously learns $\mathbf{S}$ and $\mathbf{H}$
- Problem formulated as a non-convex optimization problem
  - Convex algorithm based on AM and MM techniques
  - Proposed algorithm is shown to converge to a stationary point
- Generalized to joint GF identification to deal with several GFs
- Efficient algorithm to deal with graphs with large number of nodes
- Numerical evaluation over synthetic and real-world graphs
  - Code: `https://github.com/reysam93/graph_denoising`

Questions at: **samuel.rey.escudero@urjc.es**