

Low Pass Graph Signal Processing: Modeling Data, Inference, and Beyond

Hoi-To Wai

Department of SEEM, The Chinese University of Hong Kong

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Dealing with Network Data

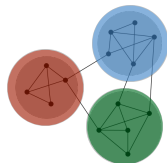
- ▶ Statistics: Gauss Markov random fields, graphical models

— *statistical association of data*



- ▶ Machine learning: dimensionality reduction

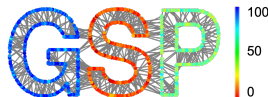
— *graph representation of data*



- ▶ **SP: Graph Signal Processing**

— *input/output association of data*

⇒ *generative, interpretable model*



Dealing with Network Data

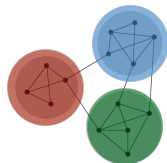
- ▶ Statistics: Gauss Markov random fields, graphical models

— *statistical association of data*



- ▶ Machine learning: dimensionality reduction

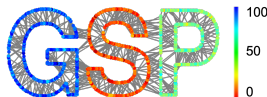
— *graph representation of data*



- ▶ **SP: Graph Signal Processing**

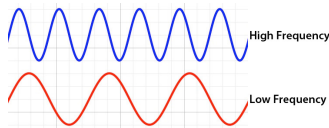
— *input/output association of data*

⇒ *generative, interpretable model*

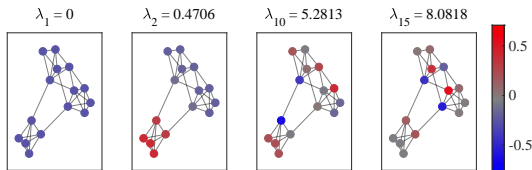


Low Pass GSP

- ▶ SP cares about the **frequency content** in a (time domain) signal — *low frequency vs high frequency*:



- ▶ Similar notion carries over to **graph signal processing (GSP)** — *low pass graph signals vs non low pass graph signals*:



Takehome Point: *Low pass* graph signals are prevalent + entail structure that enables (blind) *graph topology learning*.

Agenda

Background

Basics of GSP Models

A Quick Introduction

Low Pass Graph Signals

Graph Learning from Network Data

Smoothness and Graph Learning

Low-rank Model and Graph Feature Learning

Learning with Partial Observation

Beyond Inference Problems & Wrapping Up

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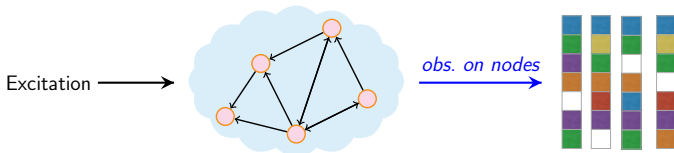
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References

Network Data = Filter + Excitation

- ▶ Consider a *undirected graph* $G = (V, E, \mathbf{A})$ with N nodes



- ▶ Graph signals = vectors defined on V , i.e., $\mathbf{x} \in \mathbb{R}^N$.

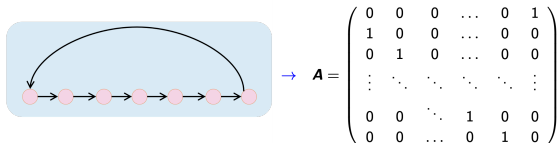
excitation $\xrightarrow{\text{'filter'}}$ signal

[†]as in SP, filter encodes the **responses** of a system to excitation.

- ▶ As SP-ers, what is our favorite form of *filter*?
- ▶ *Linear time invariant* filter = 'shifting' + 'linear combination'.

Graph Shift Operator (GSO)

- ▶ **Starting point:** Periodic signals $\mathbf{x} = (x_1, \dots, x_N)$ is 'shifted' on a cycle



$$\mathbf{A} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix} = \begin{pmatrix} x_N \\ x_1 \\ \vdots \\ x_{N-1} \end{pmatrix} \iff \text{Applying } \mathbf{A} \text{ is analogous to shifting the signal}$$

- ▶ **Generalization to graphs:** GSO mixes adjacent elements on G^1 .
- ▶ Common choice of GSO: Laplacian matrix, $\mathbf{L} = \text{Diag}(\mathbf{A}\mathbf{1}) - \mathbf{A}$.
— for the rest of the talk, we focus on **undirected** graph.
- ▶ Denote the EVD $\mathbf{L} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$ with $0 = \lambda_1 < \dots < \lambda_N$.

¹[Sandryhaila and Moura, 2013] A. Sandryhaila, J. M. Moura. Discrete signal processing on graphs. TSP, 2013; also see [Püschel and Moura, 2003].

Graph Filters

- ▶ Consider the **graph filter** as a matrix polynomial:

$$\mathcal{H}(\mathbf{L}) := \sum_{\ell=0}^{+\infty} h_{\ell} \mathbf{L}^{\ell}.$$

Shift-invariant prop: $\mathbf{y} = \mathcal{H}(\mathbf{L})\mathbf{x} \rightarrow \mathbf{L}\mathbf{y} = \mathbf{L}\mathcal{H}(\mathbf{L})\mathbf{x} \equiv \mathcal{H}(\mathbf{L})\mathbf{L}\mathbf{x}$

- ▶ **SP/GSP Perspective:** network data are **filtered** graph signals,

$$\mathbf{y} = \mathcal{H}(\mathbf{L})\mathbf{x} = \sum_{\ell=0}^{+\infty} h_{\ell} \mathbf{L}^{\ell} \mathbf{x}.$$

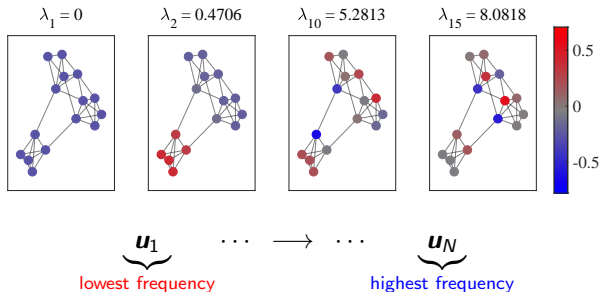
- ▶ The signal/observation is \mathbf{y} while \mathbf{x} is viewed as the **excitation**.

What are low and high frequencies basis on graph?

- ▶ High frequency graph signal \rightarrow *large variation* in adjacent entries:

$$S(\mathbf{x}) := \sum_{i,j} A_{ij} (x_i - x_j)^2 = \mathbf{x}^\top \mathbf{L} \mathbf{x}.$$

- ▶ Intuition: if $S(\mathbf{x})$ is small, the graph signal \mathbf{x} is *smooth*. It holds $S(\mathbf{u}_i) = \mathbf{u}_i^\top \mathbf{L} \mathbf{u}_i = \lambda_i$, as seen:



$\Rightarrow \mathbf{U} = (\mathbf{u}_1 \ \mathbf{u}_2 \ \cdots \ \mathbf{u}_N)$ form the right basis for graph signals on G .

Frequency Analysis via Graph Fourier Transform

- ▶ Graph Fourier Transform (GFT) calculates the frequency components of a signal:

$$\tilde{\mathbf{y}} = \mathbf{U}^T \mathbf{y} \longleftarrow \tilde{y}_i = \langle \mathbf{u}_i, \mathbf{y} \rangle.$$

- ▶ The **transfer/frequency response function** of the graph filter is:

$$\tilde{\mathbf{h}} = h(\boldsymbol{\lambda}) \quad \text{where} \quad \tilde{h}_i = h(\lambda_i) := \sum_{\ell} h_{\ell} \lambda_i^{\ell}.$$

- ▶ We have the convolution theorem:

$$\mathbf{y} = \mathcal{H}(\mathbf{L})\mathbf{x} \iff \tilde{\mathbf{y}} = \tilde{\mathbf{h}} \odot \tilde{\mathbf{x}} \quad \leftarrow \odot \text{ is element-wise product.}$$

- ▶ Graph filter can be classified as either **low-pass**², **band-pass**, or **high-pass**, depending on its graph frequency response, also see³.

²E.g., an ideal low-pass $\tilde{h}_1, \dots, \tilde{h}_K = 1, \tilde{h}_{K+1}, \dots, \tilde{h}_N = 0$.

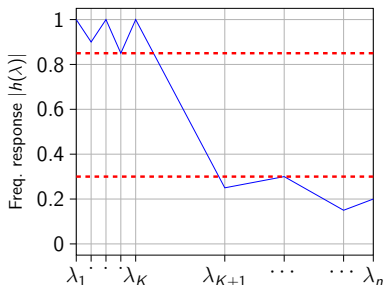
³[Isufi et al., 2022] E. Isufi, F. Gama, D. I Shuman, S. Segarra. Graph Filters for Signal Processing and Machine Learning on Graphs. ArXiv, 2022.

Low Pass Graph Filter (LPGF)

Def. For $1 \leq K \leq N - 1$, define

$$\eta_K := \frac{\max\{|h(\lambda_{K+1})|, \dots, |h(\lambda_N)|\}}{\min\{|h(\lambda_1)|, \dots, |h(\lambda_K)|\}}.$$

If the low-pass ratio satisfies $\eta_K < 1$, then $\mathcal{H}(\mathbf{L})$ is **K -low-pass**.



- ▶ Integer **K** characterizes the *bandwidth*, or the cut-off frequency.
- ▶ We say that **\mathbf{y}** is **K low pass signal** provided that $\mathbf{y} = \mathcal{H}(\mathbf{L})\mathbf{x}$, where $\mathcal{H}(\mathbf{L})$ is **K -low pass** & \mathbf{x} satisfies some mild cond..
- ▶ Graph frequencies are **non-uniformly** distributed: $\lambda_K \ll \lambda_{K+1}$ tends to induce **K -low-pass** filters, e.g., stochastic block model (SBM).

Physical Models lead to Low Pass Signals

Social Network Opinions⁴

- ▶ V = individuals, E = friends.
- ▶ DeGroot model for opinions:
$$\mathbf{y}_{t+1} = (1 - \beta)(\mathbf{I} - \alpha\mathbf{L})\mathbf{y}_t + \beta\mathbf{x}_t.$$
- ▶ **Observed** steady state:

$$\mathbf{y}_\infty = (\mathbf{I} + \tilde{\alpha}\mathbf{L})^{-1} \mathbf{x} = \mathcal{H}(\mathbf{L})\mathbf{x},$$

where $\tilde{\alpha} = \beta(1 - \alpha)/\alpha > 0$.

Prices in Stock Market⁵

- ▶ V = financial inst., E = ties.
- ▶ Business performances evolve as:
$$\mathbf{y}_{t+1} = (1 - \beta)\mathcal{H}(\mathbf{L})\mathbf{y}_t + \beta\mathbf{B}\mathbf{x},$$

e.g., stock return.
- ▶ **Observed** steady state:

$$\begin{aligned}\mathbf{y}_\infty &= \left(\frac{1}{\beta}\mathbf{I} - \frac{\bar{\beta}}{\beta}\mathcal{H}(\mathbf{L})\right)^{-1} \mathbf{B}\mathbf{x} \\ &= \tilde{\mathcal{H}}(\mathbf{L})\mathbf{B}\mathbf{x}.\end{aligned}$$

Fact⁶: Both $\mathcal{H}(\mathbf{L})$, $\tilde{\mathcal{H}}(\mathbf{L})$ are **low pass** graph filters.

⁴[DeGroot, 1974] M. H. DeGroot, Reaching a consensus. JASA, 1974.

⁵[Billio et al., 2012] M. Billio et al., Econometric measures of connectedness and systemic risk in the finance and insurance sectors, Journal of Economics Finance, 2012.

⁶[Ramakrishna et al., 2020] R. Ramakrishna, H.-T., A. Scaglione. A user guide to low-pass graph signal processing and its applications. SPM, 2020.

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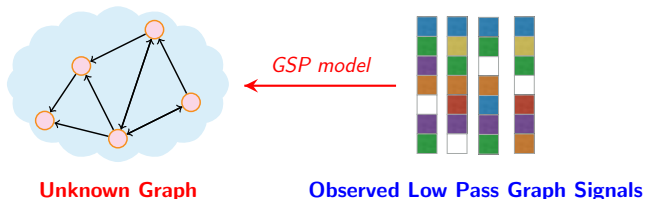
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Graph Learning from Network Data

- ▶ **Goal:** estimate \mathbf{L} or some information about it.
- ▶ **Working hypothesis:** a number of graph signals $\mathbf{y}^{(t)}$ are available as



Observed graph signals: $\mathbf{y}^{(t)} \approx \mathcal{H}(\mathbf{L})\mathbf{B}\mathbf{z}^{(t)}$, $t = 0, \dots, T - 1$
– $\mathcal{H}(\mathbf{L})$ is low pass, $\mathbf{z}^{(t)}$ is 0-mean, \mathbf{B} is **pattern** of (low rank) excitation

- ▶ Graph learning relies on **two properties** of low pass signals:
 - ▶ **Smoothness** → graph topology learning.
 - ▶ **Low-rankness** → graph feature learning (e.g., community, centrality)

Smoothness and Graph Learning

- ▶ **Insight:** For K -low-pass graph signals ($\eta_K \ll 1$) with **full-rank** excitation satisfying $\mathbf{B} = \mathbf{I}$, we observe that

$$\mathbb{E}[\mathbf{y}_\ell^\top \mathbf{L} \mathbf{y}_\ell] \approx \sum_{i=1}^K \lambda_i |h(\lambda_i)|^2 + \sigma^2 \text{Tr}(\mathbf{L}) \stackrel{\text{low pass filter}}{\approx} 0,$$

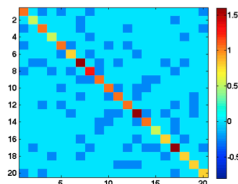
i.e., the low pass filtered graph signals are *smooth* w.r.t. \mathbf{L} .

- ▶ **Idea:** Fit a **graph** optimizing for **smoothness** (GL-SigRep)⁷:

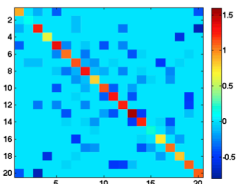
$$\begin{aligned} \min_{\mathbf{z}_\ell, \ell=1, \dots, m, \hat{\mathbf{L}}} \quad & \frac{1}{m} \sum_{\ell=1}^m \left\{ \frac{1}{\sigma^2} \|\mathbf{z}_\ell - \mathbf{y}_\ell\|_2^2 + \mathbf{z}_\ell^\top \hat{\mathbf{L}} \mathbf{z}_\ell \right\} \leftarrow \text{note } \mathbf{z} \approx \mathbf{y} \\ \text{s.t.} \quad & \text{Tr}(\hat{\mathbf{L}}) = N, \hat{L}_{ji} = \hat{L}_{ij} \leq 0, \forall i \neq j, \hat{\mathbf{L}} \mathbf{1} = \mathbf{0}, \end{aligned}$$

⁷[Dong et al., 2016] X. Dong, D. Thanou, P. Frossard, P. Vandergheynst, “Learning Laplacian matrix in smooth graph signal representations.” TSP, 2016.

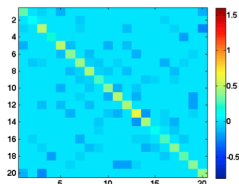
Numerical Experiment: GL-SigRep



(f) ER: Groundtruth



(g) ER: **GL-SigRep**



(h) ER: **GL-LogDet**

- ▶ Topology learnt⁸ using **GL-SigRep** from the synthetic data generated through a low pass graph filter:

$$\mathbf{y}_\ell = \sqrt{\mathbf{L}}^{-1} \mathbf{x}_\ell, \quad \mathbf{x}_\ell \sim \mathcal{N}(\mathbf{0}, \mathbf{I}),$$

- ▶ Alternative approaches:
 - ▶ [Friedman et al., 2008] Graphical LASSO: ML estimation for GMRF.
 - ▶ [Segarra et al., 2017] Spectral template: stationary graph signals.
 - ▶ [Mei and Moura, 2016] Causal modeling: time series data

⁸Image credits: [Dong et al., 2016].

Low-rank-ness and Graph Feature Learning

Issue: with low-rank excitation ($\mathbf{B} \in \mathbb{R}^{N \times R}$ with $R < N$) \rightarrow graph learning = difficult \because data is nearly rank deficient...

► **Insight:** Suppose $\mathcal{H}(\mathbf{L})$ is (η, K) **low pass**, then

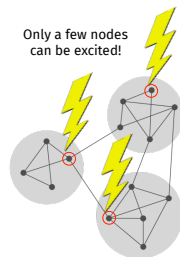
$$\mathbf{C}_y = \mathbb{E}[\mathbf{y}\mathbf{y}^\top] = \mathcal{H}(\mathbf{L})\mathbf{U}\mathbf{C}_x\mathbf{U}^\top\mathcal{H}(\mathbf{L})^\top \approx \mathbf{U}_K\mathbf{C}_{\tilde{x}}\mathbf{U}_K^\top.$$

Thus \mathbf{C}_y is also **low rank**!

► *Approximation* holds if $\eta \ll 1 \Rightarrow$ **low rank** $\mathcal{H}(\cdot)$,
 $\text{rank}(\mathcal{H}(\mathbf{L})) \approx K \ll N$ and range space $\approx \mathbf{U}_K$.

► **Idea:** spectral method to extract principal components in \mathbf{U}_K from \mathbf{C}_y .

\Rightarrow Can (still) learn **communities** and **centrality** of the graph.



Blind community detection (Blind CD)

Idea: spectral clustering applied on empirical covariance $\hat{\mathbf{C}}_y \approx \mathbf{C}_y$:

- (i) find the **top- k** $\hat{\mathbf{U}}_K \in \mathbb{R}^{N \times K}$ of $\hat{\mathbf{C}}_y = \frac{1}{m} \sum_{\ell=1}^m \mathbf{y}_\ell \mathbf{y}_\ell^\top$;
- (ii) apply **k -means** on the rows of $\hat{\mathbf{U}}_K$.

► **Theorem:** Denote the detected clusters as $\hat{\mathcal{N}}_1, \dots, \hat{\mathcal{N}}_K$, then⁹

$$\underbrace{\mathbb{K}(\hat{\mathcal{N}}_1, \dots, \hat{\mathcal{N}}_k; \mathbf{U}_K)}_{K\text{-means obj. based on } \mathbf{U}_K} - \underbrace{\mathbb{K}^*}_{\text{Optimal } K\text{-means obj.}} = \mathcal{O}(\eta_k + m^{-1/2}).$$

† \rightarrow performance of *spectral clustering* (with known topology) if $\eta_k \rightarrow 0$.

► Learning of high-level structure is **robust** to low-rank excitation.

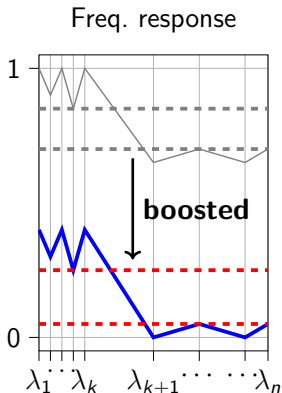
► **Extensions:** exact community recovery on multi-graphs

[Roddenberry et al., 2020], dynamic observations [Schaub et al., 2020], ...

⁹[Wai et al., 2019] H.-T., S. Segarra, A. Ozdaglar, A. Scaglione, A. Jadbabaie, "Blind community detection from low-rank excitations of a graph filter," TSP, 2019.

Blind community detection (Blind CD)

Problem: What if $\eta_K \approx 1$? Let's try $\underbrace{\tilde{\mathcal{H}}_\rho(\mathbf{L}) := \mathcal{H}(\mathbf{L}) - \rho \mathbf{I}}_{\text{'boosted' filter}} (\rho > 0)$.



▶ Original ratio: $\eta_K = \frac{0.7}{0.85} \approx 0.82$.

▶ **Boosted** ratio: $\tilde{\eta}_K = \frac{0.05}{0.25} = 0.2$.

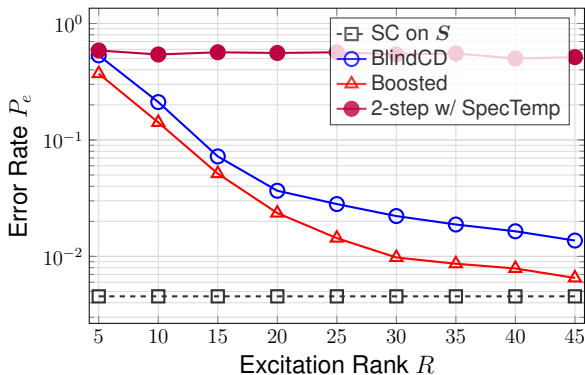
Suppose that \mathbf{Z} is known,

$$\mathbf{YZ}^\dagger = \mathcal{H}(\mathbf{L})\mathbf{B} = \underbrace{\tilde{\mathcal{H}}_\rho(\mathbf{L})\mathbf{B}}_{\text{low-rank}} + \rho\mathbf{B}$$

▶ Typically, \mathbf{B} is sparse
 \implies low-rank + sparse
 decomposition!

Robust PCA formulation: $\min_{\mathbf{L}, \mathbf{B}} \|\mathbf{YZ}^\dagger - \mathbf{L} - \mathbf{B}\|_F^2 + \gamma \|\mathbf{L}\|_* + \mu \|\mathbf{B}\|_1$

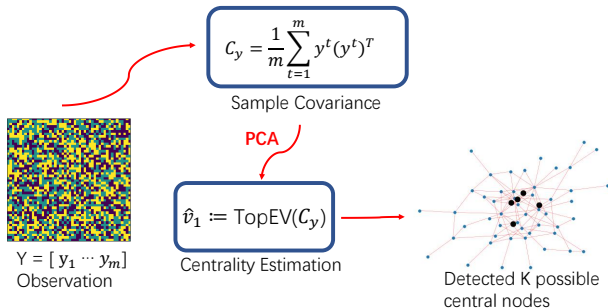
Numerical Experiment: Blind CD (+Boosting)



- (a) As $R = \text{rank}(\mathbf{C}_x)$ increases, Blind CD approaches the performance of spectral clustering on the true GSO.

Blind Centrality Learning

- ▶ Eigen-centrality = $\text{TopEV}(\mathbf{A})$ is revealed by $\text{TopEV}(\mathbf{C}_y)$ for **1-low pass** signals \implies a simple PCA procedure suffices:



- ▶ **Theorem**¹⁰: let \mathbf{v}_1 be the true eig. centrality,

$$\|\hat{\mathbf{v}}_1 - \mathbf{u}_1\|_2 = \mathcal{O}(\eta_1 + m^{-1/2}).$$

¹⁰[He and Wai, 2022] Y. He, H.-T., "Detecting central nodes from low-rank excited graph signals via structured factor analysis," TSP, 2022 \leftarrow note $\text{GSO} = \mathbf{A}$ in this case.

Blind Centrality Learning (cont'd)

- ▶ To obtain a robust formulation against $\eta_1 \approx 1$, assume that \mathbf{B} is *sparse* and use similar idea as Blind CD:

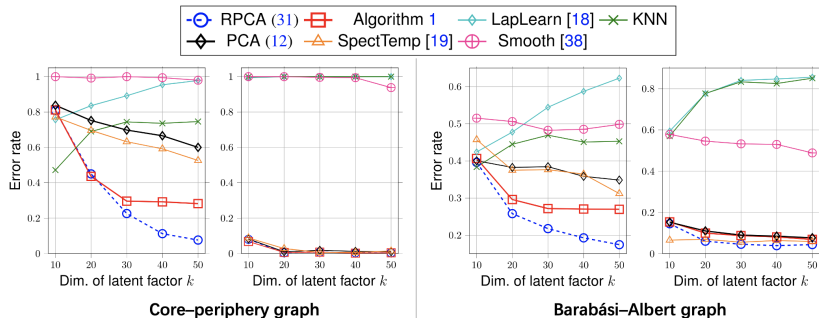
$$\begin{aligned}\mathbf{Y} &= \mathcal{H}(\mathbf{A})\mathbf{B}\mathbf{Z} = ((\mathcal{H}(\mathbf{A}) - \rho\mathbf{I})\mathbf{B} + \rho\mathbf{B})\mathbf{Z} \\ &= (\text{Low-rank} + \text{Sparse}) \times \mathbf{Z}\end{aligned}$$

- ▶ **Structured factor analysis:** if \mathbf{Z} is *unknown*,

Step 1. decompose \mathbf{Y} via **NMF**, Step 2. **Robust PCA**.

- ▶ **Theoretical analysis** (for NMF): good performance if (i) $N/\text{rank}(\mathbf{Z})$ is large, (ii) $\text{rank}(\mathbf{Z})$ is large.
 - trade-off between low-pass-ness and NMF performance.
 - derived from [Fu et al., 2019].
- ▶ **Related Works:** centrality ranking [Roddenberry and Segarra, 2021].

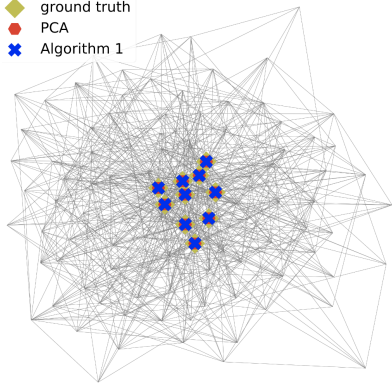
Numerical Experiment: Blind Centrality Learning



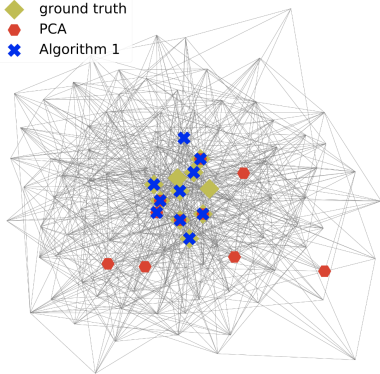
- ▶ Graph filter $\mathcal{H}(\cdot)$ is (left) 'weak' low pass, i.e., $\eta \approx 1$; (right) 'strong' low pass, i.e., $\eta \ll 1$.
- ▶ Proposed **Algorithm 1** with NMF outperforms SOTA in the considered setting for 'weak' low pass; and similarly as PCA for 'strong' low pass.

Numerical Experiment: Blind Centrality Learning

◆ ground truth
● PCA
✕ Algorithm 1



◆ ground truth
● PCA
✕ Algorithm 1



(left) 'Strong' low pass, (right) 'Weak' low pass

Numerical Experiment: Blind Centrality Learning

(a) Stock Dataset[†]

Method	Top-10 Estimated Central Stocks (sorted left-to-right)									
Algorithm 1	ALL	ACN	HON	AXP	IBM	DIS	ORCL	MMM	BRK.B	COST
	0.43	0.56	0.51	0.72	0.50	0.36	0.70	0.33	0.52	0.64
	Average Correlation Score: 0.53 ± 0.133									
PCA (11)	NVDA	NFLX	AMZN	ADBE	PYPL	CAT	MA	GOOG	BA	GOOGL
	0.56	0.60	0.68	0.63	0.65	0.27	0.67	0.63	0.28	0.63
	Average Correlation Score: 0.56 ± 0.154									
GL-SigRep [13]	GOOGL	GOOG	LLY	USB	EMR	DUK	ORCL	GD	VZ	V
	0.63	0.63	0.17	0.43	0.59	0.11	0.70	0.53	0.27	0.71
	Average Correlation Score: 0.48 ± 0.22									
KNN	ACN	HON	ALL	BRK.B	IBM	AXP	EMR	MMM	CSCO	XOM
	0.56	0.51	0.43	0.52	0.50	0.72	0.59	0.33	0.63	0.55
	Average Correlation Score: 0.53 ± 0.107									
SpecTemp [14]	ACN	ORCL	PG	LLY	SUBX	PYPL	MDLZ	FB	PFE	MRK
	0.56	0.70	0.36	0.17	0.58	0.65	0.41	0.61	0.14	0.20
	Average Correlation Score: 0.44 ± 0.211									
Kalofolias [44]	ACN	HON	BRK.B	ALL	AXP	IBM	XOM	KO	USB	COST
	0.56	0.51	0.52	0.43	0.72	0.50	0.55	0.32	0.43	0.64
	Average Correlation Score: 0.52 ± 0.112									
	Information Technology/ Communication Services/ Industrials/ Financials/ other sectors.									

(b) Senate Dataset[†]

Method	Top-10 Estimated Central States (sorted left-to-right)									
Algorithm 1	MI	MT	KS	RI	TN	MN	NV	ME	MD	IN
	0.79	0.66	0.74	0.67	0.68	0.74	0.43	0.67	0.6	0.62
	Average Correlation Score: 0.66 ± 0.099									
PCA (11)	CA	DE	CO	IL	ND	WV	IA	VA	WY	MA
	0.55	0.46	0.54	0.63	0.72	0.52	0.51	0.56	0.59	0.58
	Average Correlation Score: 0.57 ± 0.072									
GL-SigRep [13]	CA	DE	WV	CO	IL	VA	ND	IA	WY	AZ
	0.55	0.46	0.52	0.54	0.63	0.56	0.72	0.51	0.59	0.31
	Average Correlation Score: 0.54 ± 0.108									
KNN	ND	CA	IL	WV	DE	VA	AZ	CO	WY	IA
	0.72	0.55	0.63	0.52	0.46	0.56	0.31	0.54	0.59	0.51
	Average Correlation Score: 0.54 ± 0.108									
SpecTemp [14]	AL	ND	WV	CA	DE	IL	MO	MA	VA	SD
	0.61	0.72	0.52	0.55	0.46	0.63	0.57	0.58	0.56	0.56
	Average Correlation Score: 0.58 ± 0.069									
Kalofolias [44]	AL	AK	AZ	AR	WV	VA	CA	CO	CT	DE
	0.61	0.63	0.31	0.47	0.52	0.56	0.55	0.54	0.45	0.46
	Average Correlation Score: 0.51 ± 0.093									
	Republican/ Democrat/ Mixed.									

[†]The number below each stock/state shows its normalized correlation score with the S&P100 index and number of ‘Yay’s in the voting result [cf. (36)]. The average correlation scores are taken over the set of central nodes found and the number after ‘±’ is the standard deviation.

(a) Detected central nodes with performance measured on correlation of nodes with (left) S&P500 index, (right) voting outcomes.

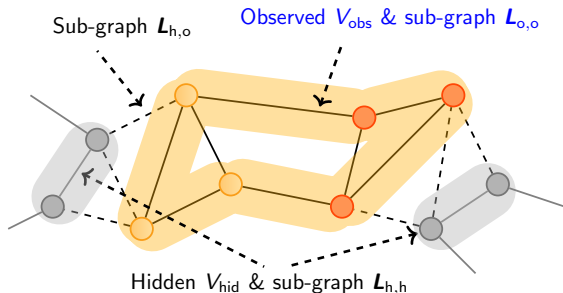
Extension: *Multiple graph learning from streaming data*¹¹.

¹¹[He and Wai, 2023b] Y. He, H.-T., “Online Inference for Mixture Model of Streaming Graph Signals with Non-White Excitation”, TSP, 2023.

Leveraging Low-passness with Partial Observation

- ▶ In many settings, we do not observe **complete graph signals** on every nodes, e.g., **large social network**, **power network**, etc.
- ▶ Hidden nodes remain **influential** and affect the **observations**:

$$\mathbf{y} = \mathcal{H}(\mathbf{L})\mathbf{x} \quad \text{with} \quad \mathbf{y} = \begin{bmatrix} \mathbf{y}_{\text{obs}} \\ \mathbf{y}_{\text{hid}} \end{bmatrix}, \quad \mathbf{L} = \begin{bmatrix} \mathbf{L}_{o,o} & \mathbf{L}_{o,h} \\ \mathbf{L}_{h,o} & \mathbf{L}_{h,h} \end{bmatrix}$$



Learning with Partial Observation

- **Goal:** infer about **the subgraph of observable nodes**, $L_{o,o}$:

$$\mathbf{y} = \mathcal{H}(\mathbf{L})\mathbf{x} = \begin{bmatrix} \mathbf{y}_{\text{obs}} \\ \mathbf{y}_{\text{hid}} \end{bmatrix}, \quad \mathbf{C}_y = \begin{bmatrix} \mathbf{C}_y^o & \mathbf{C}_y^{o,h} \\ \mathbf{C}_y^{h,o} & \mathbf{C}_y^h \end{bmatrix}, \quad \mathbf{L} = \begin{bmatrix} \boxed{L_{o,o}} & L_{o,h} \\ L_{h,o} & L_{h,h} \end{bmatrix}$$

I. Leveraging Smoothness: observing that¹²

$$\frac{1}{m} \sum_{\ell=1}^m \mathbf{y}_\ell^\top \mathbf{L} \mathbf{y}_\ell \approx \text{Tr}(\mathbf{C}_y^o \mathbf{L}_{o,o}) + \underbrace{\text{Tr}(2\mathbf{C}_y^{o,h} \mathbf{L}_{o,h}^\top)}_{\text{low rank if } |V_{\text{hid}}| \ll N} + \underbrace{\text{Tr}(\mathbf{C}_y^h \mathbf{L}_{h,h})}_{\geq 0} \geq 0$$

$$\begin{aligned} \implies \min_{L_{o,o}, K, R} & \quad \text{Tr}(\mathbf{C}_y^o \mathbf{L}_{o,o}) + \text{Tr}(\mathbf{K}) + \text{Tr}(\mathbf{R}) + \alpha g(\mathbf{L}_{o,o}) + \gamma \|\mathbf{K}\|_* \\ \text{s.t.} & \quad \text{Tr}(\mathbf{C}_y^o \mathbf{L}_{o,o}) + \text{Tr}(\mathbf{K}) + \text{Tr}(\mathbf{R}) \geq 0, \quad \text{Tr}(\mathbf{R}) \geq 0, \quad \mathbf{L}_{o,o} \in \mathcal{L}, \end{aligned}$$

where $g(\cdot)$, \mathcal{L} are respectively regularization, constraint for $L_{o,o}$ to be a proper sub-matrix of Laplacian.

¹²[Buciulea et al., 2022] A. Buciulea, S. Rey, A. G. Marques. Learning graphs from smooth and graph-stationary signals with hidden variables. TSIPN, 2022.

Learning with Partial Observation

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$$\begin{aligned} \implies \min_{\mathbf{L}_{o,o}, \mathbf{K}, \mathbf{R}} & \quad \text{Tr}(\mathbf{C}_y^o \mathbf{L}_{o,o}) + \text{Tr}(\mathbf{K}) + \text{Tr}(\mathbf{R}) + \alpha g(\mathbf{L}_{o,o}) + \gamma \|\mathbf{K}\|_* \\ \text{s.t.} & \quad \text{Tr}(\mathbf{C}_y^o \mathbf{L}_{o,o}) + \text{Tr}(\mathbf{K}) + \text{Tr}(\mathbf{R}) \geq 0, \quad \text{Tr}(\mathbf{R}) \geq 0, \quad \mathbf{L}_{o,o} \in \mathcal{L}, \end{aligned}$$

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II. Leveraging Lowrank-ness: provided $\mathcal{H}(\mathbf{L})$ is (η, K) low pass,

$$\mathbf{C}_y^o = \mathbf{E}_o \mathbf{C}_y \mathbf{E}_o^\top \approx (\mathbf{E}_o \mathbf{U}_K) \mathbf{C}_{\bar{x}} (\mathbf{E}_o \mathbf{U}_K)^\top$$

where \mathbf{E}_o is **row-selection** matrix for V_{obs} . \uparrow can estimate $\mathbf{E}_o \mathbf{U}_K \approx \mathbf{U}_{K,o}$

- ▶ **Key observation:** low-rankness of $\mathcal{H}(\mathbf{L})$ **supersedes** partial obs.
- ▶ Straightforward extension for graph feature learning: **partial community detection**¹², **partial centrality inference**¹³

¹²[Wai et al., 2022] H.-T., Y. Eldar, A. Ozdaglar, A. Scaglione, "Community Inference From Partially Observed Graph Signals: Algorithms and Analysis", TSP, 2022.

¹³[He and Wai, 2023a] Y. He, H.-T., Central nodes detection from partially observed graph signals, in ICASSP 2023.

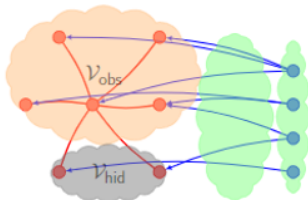
Complete Learning with Partial Observation

- ▶ **Goal:** inferring the graph features of **the whole \mathbf{A}** ,

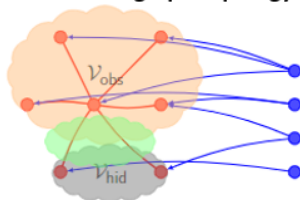
$$\mathbf{y} = \mathcal{H}(\mathbf{A})\mathbf{x} = \begin{bmatrix} \mathbf{y}_{\text{obs}} \\ \mathbf{y}_{\text{hid}} \end{bmatrix}, \mathbf{C}_y = \begin{bmatrix} \mathbf{C}_y^{\text{o}} & \mathbf{C}_y^{\text{o,h}} \\ \mathbf{C}_y^{\text{h,o}} & \mathbf{C}_y^{\text{h}} \end{bmatrix}, \mathbf{A} = \begin{bmatrix} \mathbf{A}_{\text{o,o}} & \mathbf{A}_{\text{o,h}} \\ \mathbf{A}_{\text{h,o}} & \mathbf{A}_{\text{h,h}} \end{bmatrix}$$

- ▶ Requires *side information* or *sub-graph topology*:

Known side information



Known sub-graph topology



- ▶ We rely on *low-rankness* and aim to learn community or centrality.

Complete Learning with Partial Observation

- ▶ **Goal:** inferring the graph features of **the whole \mathbf{A}** ,

$$\mathbf{y} = \mathcal{H}(\mathbf{A})\mathbf{x} = \begin{bmatrix} \mathbf{y}_{\text{obs}} \\ \mathbf{y}_{\text{hid}} \end{bmatrix}, \mathbf{C}_y = \begin{bmatrix} \mathbf{C}_y^{\text{o}} & \mathbf{C}_y^{\text{o,h}} \\ \mathbf{C}_y^{\text{h,o}} & \mathbf{C}_y^{\text{h}} \end{bmatrix}, \mathbf{A} = \begin{bmatrix} \mathbf{A}_{\text{o,o}} & \mathbf{A}_{\text{o,h}} \\ \mathbf{A}_{\text{h,o}} & \mathbf{A}_{\text{h,h}} \end{bmatrix}$$

- ▶ Requires *side information or sub-graph topology*:

(I) If $\mathbf{A}_{\text{o,h}}$ is known¹⁴: Nyström method [Fowlkes et al., 2004] to 'interpolate' eigenvectors,

$$(i) \text{ top-}K \hat{\mathbf{U}}_K \text{ of } \hat{\mathbf{C}}_y^{\text{obs}}, \quad (ii) \hat{\mathbf{V}}_K := \begin{pmatrix} \hat{\mathbf{U}}_K \\ \mathbf{A}_{\text{h,o}} \hat{\mathbf{U}}_K / \hat{\lambda} \end{pmatrix}, \quad (iii) k\text{-means on } \hat{\mathbf{V}}_K.$$

- ▶ Assume that V_{obs} is chosen at random, then w.h.p.,

$$\underbrace{F(\hat{\mathcal{N}}_1, \dots, \hat{\mathcal{N}}_k; \mathbf{V}_K)}_{K\text{-means obj. on whole graph.}} - F^* = \mathcal{O} \left(\eta_K + \frac{1}{\sqrt{m}} + \frac{1}{\sqrt{|V_{\text{obs}}|}} + \frac{|V_{\text{hid}}|}{|V|} \right).$$

¹⁴[Wai et al., 2022] H.-T., Y. Eldar, A. Ozdaglar, A. Scaglione, "Community Inference From Partially Observed Graph Signals: Algorithms and Analysis", TSP, 2022.

Complete Learning with Partial Observation

- ▶ **Goal:** inferring the graph features of **the whole \mathbf{A}** ,

$$\mathbf{y} = \mathcal{H}(\mathbf{A})\mathbf{x} = \begin{bmatrix} \mathbf{y}_{\text{obs}} \\ \mathbf{y}_{\text{hid}} \end{bmatrix}, \mathbf{C}_y = \begin{bmatrix} \mathbf{C}_y^{\text{o}} & \mathbf{C}_y^{\text{o,h}} \\ \mathbf{C}_y^{\text{h,o}} & \mathbf{C}_y^{\text{h}} \end{bmatrix}, \mathbf{A} = \begin{bmatrix} \mathbf{A}_{\text{o,o}} & \mathbf{A}_{\text{o,h}} \\ \mathbf{A}_{\text{h,o}} & \mathbf{A}_{\text{h,h}} \end{bmatrix}$$

- ▶ Requires *side information or sub-graph topology*:

(II) **Excitation signal is known**¹⁴: recall $\mathbf{x}^{(t)} = \mathbf{B}\mathbf{z}^{(t)}$ and we know $\mathbf{B}, \mathbf{z}^{(t)}$.

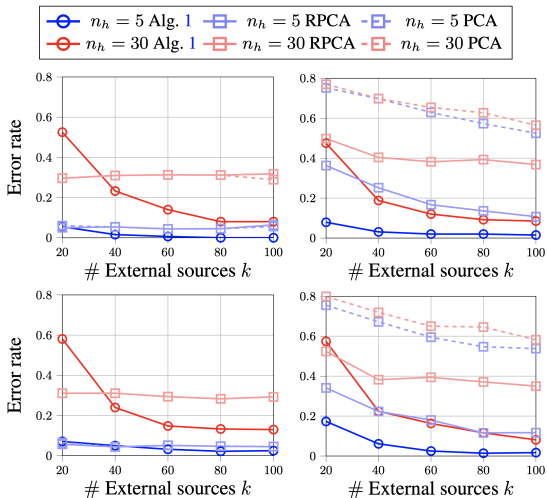
$$\mathbf{Y}_{\text{obs}}\mathbf{Z}^\dagger = \underbrace{\tilde{h}_\rho(\lambda_1)\mathbf{c}_{\text{obs}}\mathbf{c}^\top\mathbf{B}}_{\text{rank-1 w/ eig.-centrality}} + \underbrace{\rho\mathbf{E}_o\mathbf{B}}_{\text{sparse}} + \mathcal{O}(\tilde{\eta}), \quad \text{holds } \underbrace{\forall \rho > 0}_{\text{'boosting'}}$$

- ▶ **Full eigen-centrality \mathbf{c}** can be estimated if

$$\text{Excitation rank} = \text{rank}(\mathbf{B}) = K \geq |\mathbf{V}_{\text{hid}}| + 1$$

¹⁴[He and Wai, 2023a] Y. He, H.-T., Central nodes detection from partially observed graph signals, in ICASSP 2023.

Numerical Experiment: Complete Graph Learning



- Increasing the excitation rank K improves the detection performances.

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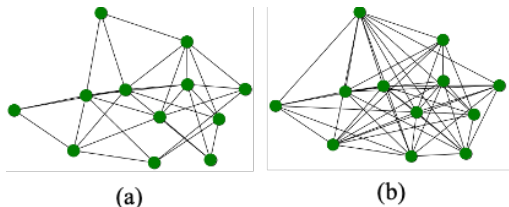
Beyond Inference Problems & Wrapping Up

References

Detecting Low-pass Signals

Question: How do we know if a set of graph signals are low pass?

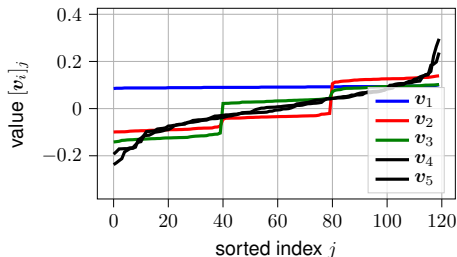
- ▶ Topology inferred from non low pass signals can be **deceptive**.



- (a) Ground truth. (b) Topology learnt by GL-SigRep on **non-low-pass** signals.
- ▶ *Challenges:* graph topology \mathbf{A} and filter $\mathcal{H}(\mathbf{A})$ are **unknown**.
- ▶ **Warning:** an **ill posed** problem – graph signals is *smooth* on one graph, but *non-smooth* on another.

Detecting Low-pass Signals

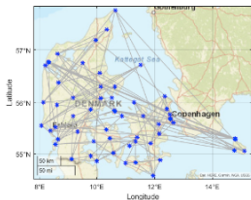
- ▶ **Assume:** no. of dense clusters, K , in the graph is known a-priori.
 $\implies \lambda_1, \dots, \lambda_K \approx 0 \implies$ if the filter is low pass, it will be K low pass.
- ▶ **Observation:** graph signals from K low pass filter exhibit particular *spectral signature*. E.g., SBM graph with $K = 3$ clusters,



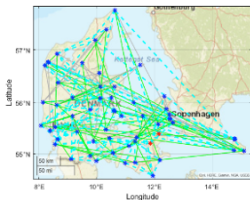
Idea: Measure *clusterability* of principal eigenvectors.

Application: Robustifying Graph Learning

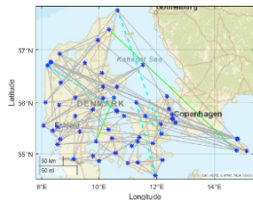
What if graph signals are corrupted with non-low-pass observations? \implies **screen them out** by a blind detector and apply [Dong et al., 2016].



(a)



(b)



(c)

- (a) Ground truth graph learnt from clean data.
- (b) Graph learnt from **corrupted** data (mixed w/ high-pass signals).
- (c) Graph learnt after the **pre-screening** procedure.

► **Other applications:** blind detection of network dynamics, blind anomaly detection, etc.¹⁵

¹⁵[Zhang et al., 2023a] C. Zhang, Y. He, H.-T.. Detecting Low Pass Graph Signals via Spectral Pattern: Sampling Complexity and Applications. ArXiv, 2023.

Stability of Graph Filter with Edge Rewiring

- ▶ Graph filter is an important building block of *Graph Convolutional Neural Network (GCN)* \rightarrow trained on $\mathcal{H}(\mathbf{L})$, but applied on $\mathcal{H}(\hat{\mathbf{L}})$.
- ▶ **Stability**¹⁶ is related to *transferability* of GCNs. Existing results require small no. of edge rewires.

Frequency-domain bound: If $\mathcal{H}(\mathbf{L})$ is **low pass**, then

$$\|\mathcal{H}(\mathbf{L}) - \mathcal{H}(\hat{\mathbf{L}})\| = \mathcal{O}(\eta + \|\mathbf{U}_k - \hat{\mathbf{U}}_k\| + \|\mathbf{\Lambda}_k - \hat{\mathbf{\Lambda}}_k\|),$$

where $\mathbf{U}_k - \hat{\mathbf{U}}_k$, $\mathbf{\Lambda}_k - \hat{\mathbf{\Lambda}}_k$ are perturbations of top eigenvectors/values.

- ▶ Residuals $\rightarrow 0$ for edge rewiring on SBMs perturbations¹⁷.
— Proof: depends on convergence of graph filter on SBM.

¹⁶[Gama et al., 2020] F. Gama, J. Bruna, A. Ribeiro. Stability properties of graph neural networks. TSP, 2020.

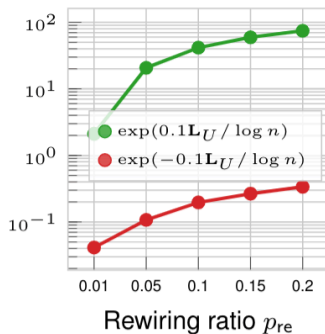
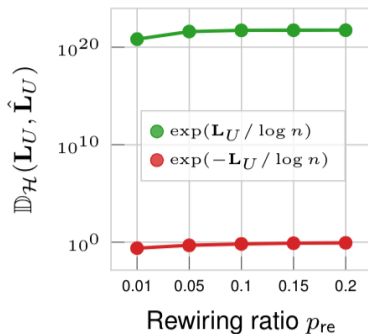
¹⁷[Nguyen et al., 2022] H. Nguyen, Y. He, H.-T., "On the stability of low pass graph filter with a large number of edge rewires," in ICASSP, 2022.

Stability of Graph Filter with Edge Rewiring

Frequency-domain bound: If $\mathcal{H}(\mathbf{L})$ is **low pass**, then

$$\|\mathcal{H}(\mathbf{L}) - \mathcal{H}(\hat{\mathbf{L}})\| = \mathcal{O}(\eta + \|\mathbf{U}_k - \hat{\mathbf{U}}_k\| + \|\mathbf{\Lambda}_k - \hat{\mathbf{\Lambda}}_k\|),$$

where $\mathbf{U}_k - \hat{\mathbf{U}}_k$, $\mathbf{\Lambda}_k - \hat{\mathbf{\Lambda}}_k$ are perturbations of top eigenvectors/values.



► **Low pass filters** are *insensitive* to no. of rewiring vs. **high pass filters**.

Generalization Bound

- ▶ **Sample complexity** of MPNN (GCN) learning¹⁸ analyzed via

$$\mathcal{E}_m^n = \mathbb{E}_{\mu_G^m} \left[\sup_{\Theta} \left(\underbrace{\frac{1}{m} \sum_{i=1}^m \mathcal{L}(\Theta_{G^i}(\mathbf{x}^i), \mathbf{y}^i)}_{\text{empirical risk}} - \underbrace{\mathbb{E}_{\mu_G}[\mathcal{L}(\Theta_G(\mathbf{x}), \mathbf{y})]}_{\text{expected risk}} \right)^2 \right] \leq \frac{C}{m} n^{-\frac{1}{D_{\mathcal{X}}+1}}$$

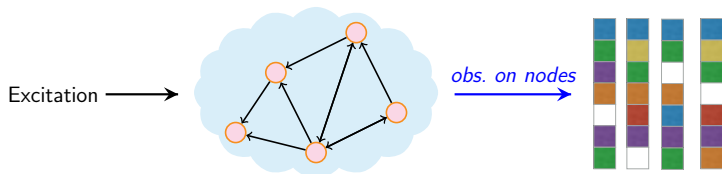
where m = no. of training sets, n = no. of nodes, and $G^i, \mathbf{x}^i, \mathbf{y}^i$ is the i th training set of graph, attributes (signals), labels.

- ▶ **Proof:** MPNN \rightarrow graphon limit as $n \rightarrow \infty$ [Keriven et al., 2020].
- ▶ C depends on Lipschitz-ness of message (activation) functions, etc. \leftarrow no explicit dependence on graph filter.
- ▶ Recent work¹⁹ provide transferability bound utilizing the spectrum of graph filter similar to [Keriven et al., 2020] \leftarrow *open problem?*

¹⁸[Maskey et al., 2022] S. Maskey, R. Levie, Y. Lee, and G. Kutyniok. Generalization analysis of message passing neural networks on large random graphs. in NeurIPS, 2022.

¹⁹[Ruiz et al., 2021] L. Ruiz, L. F. Chamon, A. Ribeiro. Transferability properties of graph neural networks. ArXiv, 2021

Wrapping Up



- ▶ **Takehome Point:** *Low pass* graph signals are prevalent + entail structure that enables (blind) *graph topology learning*.
 - ▶ **Smoothness** → graph topology learning.
 - ▶ **Low-rankness** → topology **feature** learning (centrality, community).
 - ▶ also for learning from partial observation, ...
- ▶ Related problems: how to detect low pass signals, application to graph ML, ...

Perspectives

- ▶ Graph learning from partial observations with **many hidden nodes**.
— it is the case for observations on social/economics networks.
- ▶ Learning from **multi-attribute signal**: graphs do not live in isolation, e.g., multiplex networks in ecology, social systems, etc.
— needs new notion for graph filter:

$$\text{Prod-Graph Filter : } \mathcal{H}(\mathbf{L}^C, \mathbf{L}^G) = \sum_{i,j} h_{ij}(\mathbf{L}^C)^i \otimes (\mathbf{L}^G)^j,$$

and **interpretation** for low pass multi-layer graph filter

[Zhang et al., 2023b, Kadambari and Chepuri, 2021, Einizade and Sardouie, 2022].

Thank you!
Questions & comments are welcomed.

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