Learning graphs from data: A signal processing perspective

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#### # samples M

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Input: fMRI recordings in these regions



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#### How do we build/learn the graph?

image credit: http://blog.myesr.org/mri-reveals-the-human-connectome/ https://www.iconexperience.com

#### Outline

- A (partial) historic overview
- A signal processing perspective
  - GSP idea for graph learning
  - Three signal/graph models
- Perspective

- Simple and intuitive methods
  - Sample correlation
  - Similarity function (e.g., Gaussian RBF)

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Undirected graphical models: Markov random fields (MRF)

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$$(i,j) \notin E \Leftrightarrow x_i \perp x_j \mid \mathbf{x} \setminus \{x_i, x_j\}$$



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probability parameterized by  $\boldsymbol{\Theta}$  :

$$P(\mathbf{x}|\mathbf{\Theta}) = \frac{1}{Z(\mathbf{\Theta})} \exp\left(\sum_{i \in V} \theta_{ii} x_i^2 + \sum_{(i,j) \in E} \theta_{ij} x_i x_j\right)$$

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Gaussian graphical models with precision  $\boldsymbol{\Theta}$  :

$$P(\mathbf{x}|\mathbf{\Theta}) = \frac{|\mathbf{\Theta}|^{1/2}}{(2\pi)^{N/2}} \exp\left(-\frac{1}{2}\mathbf{x}^T\mathbf{\Theta}\mathbf{x}\right)$$

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Learning a sparse  $\Theta$  :

- interactions are mostly local
- computationally more tractable

covariance selection			
Dempster			
1972			

Prune the smallest elements in precision (inverse covariance) matrix



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Not applicable when sample covariance is not invertible!



Learning a graph = learning neighborhood of each node







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LASSO regression:

 $\min_{\boldsymbol{\beta}_1} ||\mathbf{X}_1 - \mathbf{X}_{\backslash 1}\boldsymbol{\beta}_1||^2 + \lambda ||\boldsymbol{\beta}_1||_1$ 



#### Estimation of sparse precision matrix





Estimation of sparse precision matrix





graphical LASSO maximizes likelihood of precision matrix  $\boldsymbol{\Theta}$  :

$$\mathbf{\Theta}|^{M/2} \exp\left(-\sum_{m=1}^{M} \frac{1}{2} \mathbf{X}(m)^T \mathbf{\Theta} \mathbf{X}(m)\right)$$



Estimation of sparse precision matrix



graphical LASSO maximizes likelihood of precision matrix  $\boldsymbol{\Theta}$  :

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log-likelihood function



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Neighborhood learning for discrete variables







#### Neighborhood learning for discrete variables







Neighborhood learning for discrete variables





regularized logistic regression:

$$\max_{\boldsymbol{\beta}_1} \log P_{\boldsymbol{\beta}}(\mathbf{X}_{1m}|\mathbf{X}_{\backslash 1m}) - \lambda ||\boldsymbol{\beta}_1||_1$$

logistic function

- Simple and intuitive methods
  - Sample correlation
  - Similarity function (e.g., Gaussian RBF)
- Learning graphical models
  - Classical learning approaches lead to both positive/negative relations
  - What about learning a graph topology with non-negative weights?
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#### From arbitrary precision matrix to graph Laplacian!



$$\max_{\boldsymbol{\Theta}} \log \det \boldsymbol{\Theta} - \operatorname{tr}(\mathbf{S}\boldsymbol{\Theta}) - \rho ||\boldsymbol{\Theta}||_1$$

graph Laplacian  ${\rm L}$  can be the precision, BUT it is singular













- Existing approaches have limitations
  - Simple correlation or similarity functions are not enough
  - Most classical methods for learning graphical models do not directly lead to topologies with non-negative weights
  - There is no strong emphasis on signal/graph interaction with spectral/frequencydomain interpretation

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  - Simple correlation or similarity functions are not enough
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  - There is no strong emphasis on signal/graph interaction with spectral/frequencydomain interpretation
- Opportunity and challenge for graph signal processing
  - GSP tools such as frequency-analysis and filtering can contribute to the graph learning problem
  - Filtering-based approaches can provide generative models for signals with complex non-Gaussian behavior

• Signal processing is about  $\mathbf{D} \mathbf{c} = \mathbf{x}$ 



- Graph signal processing is about  $\mathsf{D}(\mathsf{G}) \ \mathsf{c} = \mathsf{x}$ 



• Forward: Given  ${\bm G}$  and  ${\bm x},$  design  ${\bm D}$  to study  ${\bm c}$ 



trained dictionary atoms graph dictionary

graph dictionary coefficient [Zhang12,Thanou14]

- Backward (graph learning): Given  $\boldsymbol{x}$ , design  $\boldsymbol{D}$  and  $\boldsymbol{c}$  to infer  $\boldsymbol{G}$ 



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- The key is a signal/graph model behind **D**
- Designed around graph operators (adjacency/Laplacian matrices, shift operators)
- Choice of/assumption on **c** often determines signal characteristics

- Signal values vary smoothly between all pairs of nodes that are connected
- Example: Temperature of different locations in a flat geographical region
- Usually quantified by the Laplacian quadratic form:

$$\mathbf{x}^{T}\mathbf{L}\mathbf{x} = \frac{1}{2}\sum_{i,j} \mathbf{W}_{ij} \left(\mathbf{x}(i) - \mathbf{x}(j)\right)^{2}$$

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$$\mathbf{x} : V \to \mathbb{R}^{N}$$

$$\mathbf{x}_{i,j} = 1$$

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#### Similar to previous approaches:

Lake (2010): 
$$\max_{\boldsymbol{\Theta} = \mathbf{L} + \frac{1}{\sigma^2} \mathbf{I}} \log \det \boldsymbol{\Theta} - \frac{1}{M} \operatorname{tr}(\mathbf{X}\mathbf{X}^T \boldsymbol{\Theta}) - \rho ||\boldsymbol{\Theta}||_1$$
  
Daitch (2009): 
$$\min_{\mathbf{L}} \mathbf{X}^T \mathbf{L}^2 \mathbf{X}$$
  
Hu (2013): 
$$\min_{\mathbf{L}} \operatorname{tr}(\mathbf{X}^T \mathbf{L}^s \mathbf{X}) - \beta ||\mathbf{W}||_F$$



- Dong et al. (2015) & Kalofolias (2016)
  - $\mathbf{D}(\mathcal{G}) = \boldsymbol{\chi}$  (eigenvector matrix of L)
  - Gaussian assumption on  $c{:}~c\sim\mathcal{N}(0,\Lambda)$



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 Maximum a posterior (MAP) estimation on c leads to minimization of Laplacian quadratic form:

$$\begin{split} \min_{c} ||\mathbf{x} - \boldsymbol{\chi} \mathbf{c}||_{2}^{2} - \log P_{c}(\mathbf{c}) \\ & \downarrow \\ \\ \min_{\mathbf{L}, \mathbf{Y}} (||\mathbf{X} - \mathbf{Y}||_{F}^{2}) + \alpha (\operatorname{tr}(\mathbf{Y}^{T} \mathbf{L} \mathbf{Y}) + \beta (||\mathbf{L}||_{F}^{2}) \\ \\ & \operatorname{data fidelity} \quad \operatorname{smoothness on} \mathbf{Y} \quad \operatorname{regularization} \end{split}$$

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Learning enforces signal property (global smoothness)!





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#### **Generalizes graphical LASSO and Lake**

Adding priors on edge weights leads to interpretation of MAP estimation

• Chepuri et al. (2016)





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- An edge selection mechanism based on the same smoothness measure:



Similar in spirit to Dempster Good for learning unweighted graph Explicit edge-handler is desirable in some applications
- Signals are outcome of some diffusion processes on the graph (more of local smoothness than global one!)
- Example: Movement of people/vehicles in transportation network

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  - Two-step approach:
    - Estimate eigenvector matrix from sample covariance (if covariance unknown):

$$\boldsymbol{\Sigma} = \mathbb{E} \Big[ \sum_{m=1}^{M} \mathbf{X}(m) \mathbf{X}(m)^{T} \Big] = \sum_{m=1}^{M} \mathbf{W}_{\text{norm}}^{2\mathbf{k}(m)} \quad \text{(polynomial of } \mathbf{W}_{\text{norm}} \text{)}$$



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### More a "graph-centric" learning framework: Cost function on graph components instead of signals



• Segarra et al. (2016)

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$$\mathbf{D}(\mathcal{G}) = \mathbf{H}(\mathbf{S}_{\mathcal{G}}) = \sum_{l=0}^{L-1} h_l \mathbf{S}_{\mathcal{G}}^l$$



(diffusion defined by a graph shift operator  $S_{\mathcal{G}}$  that can be arbitrary, but practically W or L)

- **c** is a white signal

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$$\min_{\mathbf{S}_{\mathcal{G}},\lambda} ||\mathbf{S}_{\mathcal{G}}||_{0} \quad \text{s.t.} \quad \mathbf{S}_{\mathcal{G}} = \sum_{n=1}^{N} \lambda_{n} \mathbf{v}_{n} \mathbf{v}_{n}^{T} \qquad \text{``spectral templates''} (eigenvectors)$$

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Similar in spirit to Pasdeloup, same assumption on stationarity but different inference framework due to different D

Can handle noisy or incomplete information on spectral templates

- Thanou et al. (2016)
  - $\mathbf{D}(\mathcal{G}) = e^{-\tau \mathbf{L}}$  (localization in vertex domain)
  - Sparsity assumption on  ${\boldsymbol{c}}$



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Still diffusion-based model, but more "signal-centric"

No assumption on eigenvectors/stationarity, but on signal structure and sparsity Can be extended to general polynomial case (Maretic et al. 2017)



- Signals are time-varying observations that are causal outcome of current or past values (mixed degree of smoothness depending on previous states)
- Example: Evolution of individual behavior due to influence of different friends at different timestamps
- Characterized by an autoregressive model or a structural equation model (SEM)

- Mei and Moura (2015)
  - $\mathbf{D}_s(\mathcal{G}) = \mathbf{P}_s(\mathbf{W})$ : polynomial of **W** of degree s
  - Define  $\mathbf{c}_s$  as  $\mathbf{x}[t-s]$



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× )=

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 $\min_{\mathbf{W},\mathbf{a}} \frac{1}{2} \sum_{k=S+1}^{K} ||\mathbf{x}[k] - \sum_{s=1}^{S} \mathbf{P}_{s}(\mathbf{W})\mathbf{x}[k-s]||_{2}^{2} + \lambda_{1} ||\operatorname{vec}(\mathbf{W})||_{1} + \lambda_{2} ||\mathbf{a}||_{1}$ 

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 $\mathbf{x}$ 



Polynomial design similar in spirit to Pasdeloup and Segarra Good for inferring causal relations between signals Kernelized version (nonlinear): Shen et al. (2016)

- Baingana and Giannakis (2016)
  - $\mathbf{D}(\mathcal{G}) = \mathbf{W}^{\mathbf{s}(t)}$  : Graph at time  $\mathbf{t}$

(topologies switch at each time between S discrete states)

- Define **c** as **x** 



- Baingana and Giannakis (2016)
  - $\mathbf{D}(\mathcal{G}) = \mathbf{W}^{\mathbf{s}(t)}$  : Graph at time  $\mathbf{t}$

 $+ W X = U v_{2} v_{2} v_{1} v_{2} v_{2} v_{5}$ ext. W X X G

(topologies switch at each time between S discrete states)

- Define **c** as **x** 



- Baingana and Giannakis (2016)
  - $\mathbf{D}(\mathcal{G}) = \mathbf{W}^{\mathbf{s}(t)}$  : Graph at time  $\mathbf{t}$

(topologies switch at each time between S discrete states)

- Define **c** as **x** 



ext.

+

 $\mathbf{W}$ 

×

 $\mathbf{X}$ 

=

 $\mathbf{X}$ 

G

- Solve for all states of W:



- Baingana and Giannakis (2016)
  - $\mathbf{D}(\mathcal{G}) = \mathbf{W}^{\mathbf{s}(t)}$  : Graph at time  $\mathbf{t}$

(topologies switch at each time between S discrete states)

- Define **c** as **x** 



ext.

+

×

 $\mathbf{W}$ 

=

 $\mathbf{X}$ 

 $\mathbf{X}$ 

- Solve for all states of **W**:



Good for inferring causal relations between signals as well as dynamic topologies

# Comparison of different methods

Methods	Signal model	Assumption	Learning output	Edge direction	Inference
Dong (2015)	Global smoothness	Gaussian	Laplacian	Undirected	Signal-centric
Kalofolias (2016)	Global smoothness	Gaussian	Adjacency	Undirected	Signal-centric
Egilmez (2016)	Global smoothness	Gaussian	Generalized Laplacian	Undirected	Signal-centric
Chepuri (2016)	Global smoothness	Gaussian	Adjacency	Undirected	Graph-centric
Pasdeloup (2015)	Diffusion by Adj.	Stationary	Normalized Adj./ Laplacian	Undirected	Graph-centric
Segarra (2016)	Diffusion by Graph shift operator	Stationary	Graph shift operator	Undirected	Graph-centric
Thanou (2016)	Heat diffusion	Sparsity	Laplacian	Undirected	Signal-centric
Mei (2015)	Time-varying	Dependent on previous states	Adjacency	Directed	Signal-centric
Baingana (2016)	Time-varying	Dependent on current int/ext info	Time-varying Adjacency	Directed	Signal-centric





### Learning input

- missing observations
- partial observations,
  e.g., by sampling



GSP for graph learning

### Learning input

- missing observations
- partial observations,
  e.g., by sampling



- directed graphs (Shen 2017)
- time-varying graphs (Kalofolias 2017)
- multi-layer graphs
- subgraphs or
  "ego-networks"
  - intermediate graph representation



# GSP for graph learning

### Learning input

- missing observations
- partial observations,
  e.g., by sampling

### Signal/graph model

 beyond smoothness: localization in vertex-frequency domain, bandlimited (Sardellitti 2017)



- directed graphs (Shen 2017)
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### **Theoretical consideration**

- performance guarantee (Rabbat 2017)
- computational efficiency







### Learning input

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### Theoretical consideration

- performance guarantee (Rabbat 2017)
- computational efficiency

#### Learning objective

- for what SP applications? e.g., classification (Yankelevsky 2016), coding and compression (Rotondo 2015, Fracastoro 2016)
- for traditional graph-based learning, e.g., clustering, dim. reduction, ranking





### Learning input

- missing observations
- partial observations,
  e.g., by sampling

### Signal/graph model

beyond smoothness: localization in vertex-frequency domain, bandlimited (Sardellitti 2017)

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# Graph learning at GSPW 2017

#### Thursday June 1st

8:30 – 10:10		Graph Structural Analysis and Topology Identification				
8:30	8:55	Oguzhan Teke and P.P. Vaidyanathan	Discrete Uncertainty Principles and Sparse Eigenvectors	Oguzhan Teke		
8:55	9:20	Eduardo Pavez, Hilmi E. Eglimez, and Antonio Ortega	Learning Graphs with Structured Sparsity Properties: Theoretical Analysis and Algorithms	Eduardo Pavez		
9:20	9:45	Hoi-To Wai, Anna Scaglione, Amir Leshem, Sissi Xiaoxiao Wu, Uzi Harush, and Barush Barzel	Network RADAR: Theory and Practice for Network Topology Inference from Perturbation Data	Hoi-To Wai		
9:45	10:10	Paul Bogdan	Compact yet Accurate Mathematical Modeling: New Mathematical Tools for Graph Topology Inference	Paul Bogdan		

#### Friday June 2nd

8:30 – 10:35		System Identification and Statistical Processing on Graphs				
8:30	8:55	Abhishek Deb, Nagaraj T. Janakiraman, and Krishna R. Narayanan	Exploring connections between Spectral Estimation for Graph Signals, Coding Theory and Compressed Sensing	Nagaraj T. Janakiraman		
8:55	9:20	Antonio G. Marques and Santiago Segarra	Joint Inference of Multiple Networks from Stationary Graph Signals	Antonio Marques		
9:20	9:45	Rasoul Shafipour, Santiago Segarra, Antonio G. Marques and Gonzalo Mateos	Network Topology Inference from Non-Stationary Graph Signals	Gonzalo Mateos		
9:45	10:10	Fernando Gama and Alejandro Ribeiro	Optimal Graph Filter for Estimating the Mean of a WSS Graph Process	Alejandro Ribeiro		
10:10	10:35	Arman Hasanzadeh, Xi Liu, Krishna Narayanan, Nick Duffield, Byron Chigoy and Shawn Turner	Congestion Detection and Traffic Prediction in Transportation Networks Using Graph Signal Processing	Arman Hasanzadeh		

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