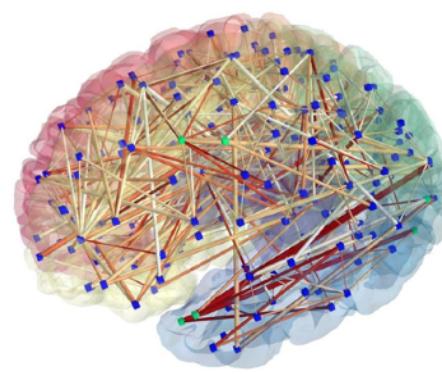
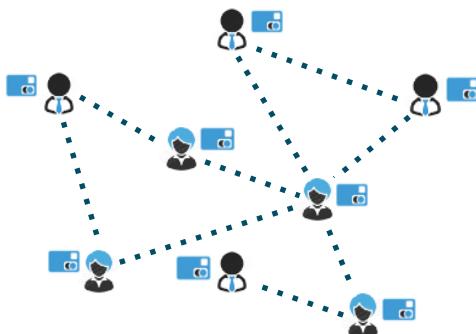
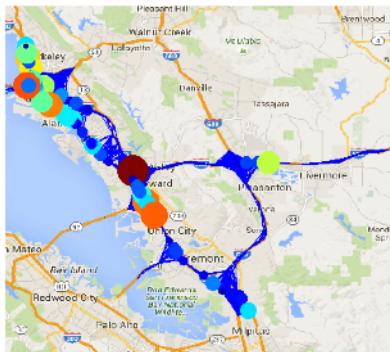




LEARNING GRAPHS FROM DATA: A GENERAL OVERVIEW

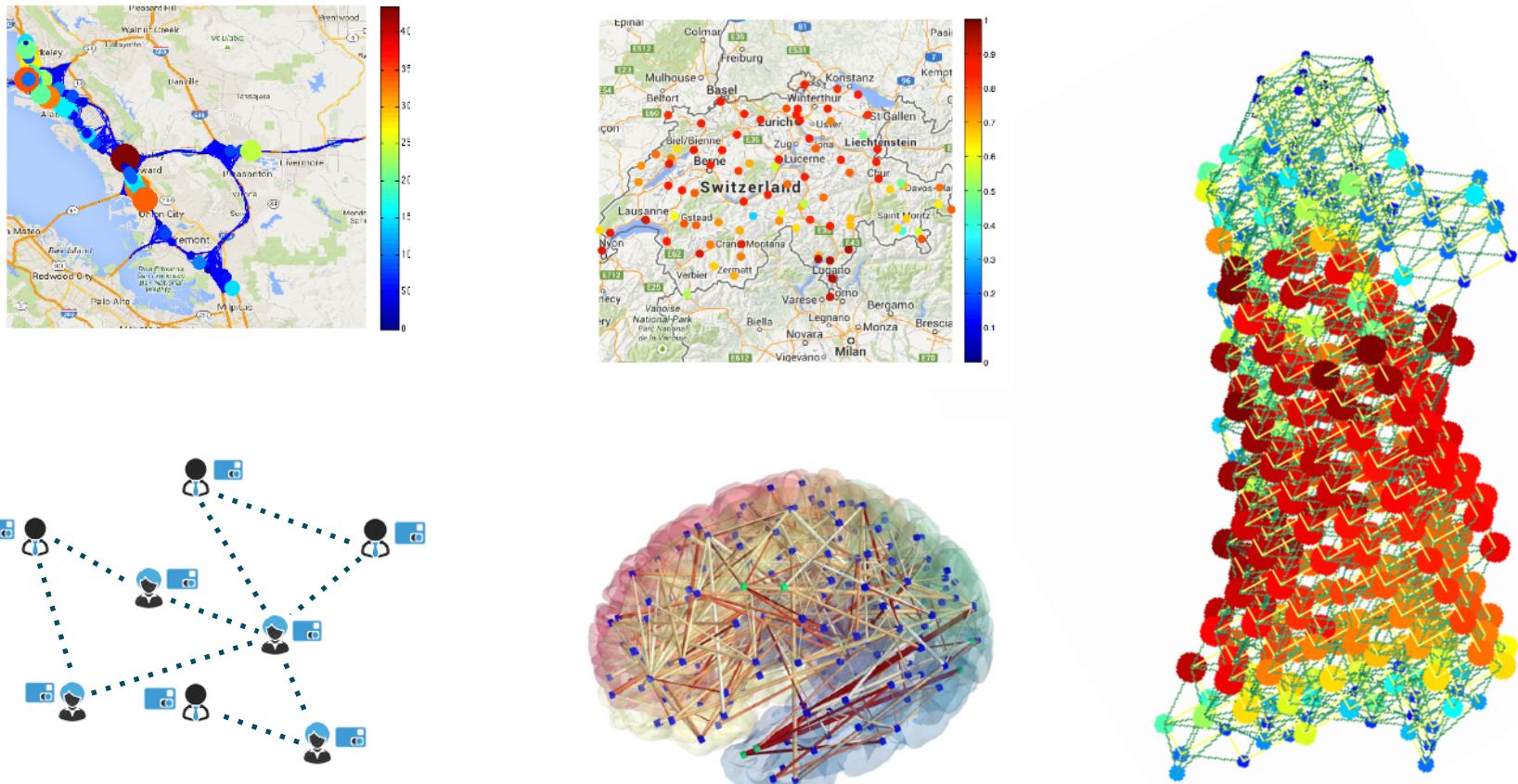
Dorina Thanou
Swiss Data Science Center (SDSC), EPFL/ETH Zurich

Data is often structured



Graphs: flexible tools to represent the geometric structure of signals defined on irregular domains

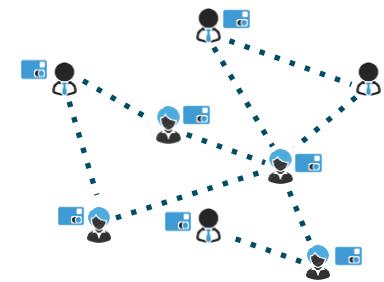
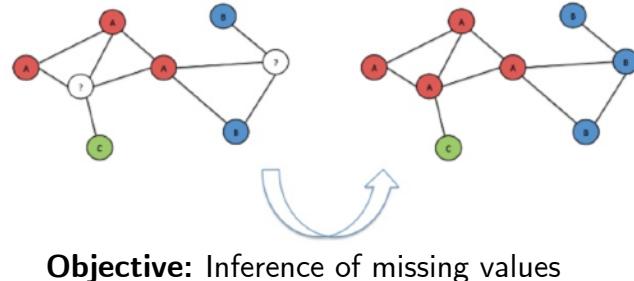
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Graphs: flexible tools to represent the geometric structure of signals defined on irregular domains

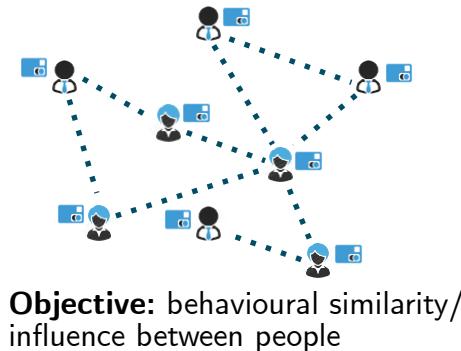
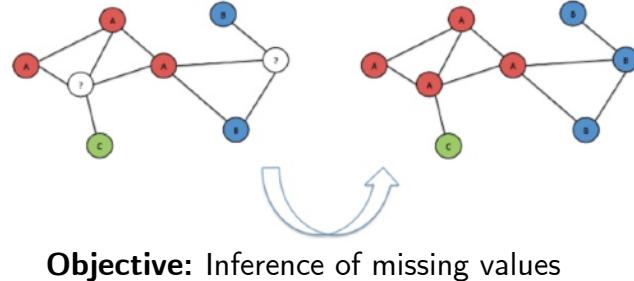
The importance of the graph

- Graph signal models define the interplay between signals and structure
 - Such models are used for **effective data processing or understanding**
 - Useful for **future prediction/decision making**



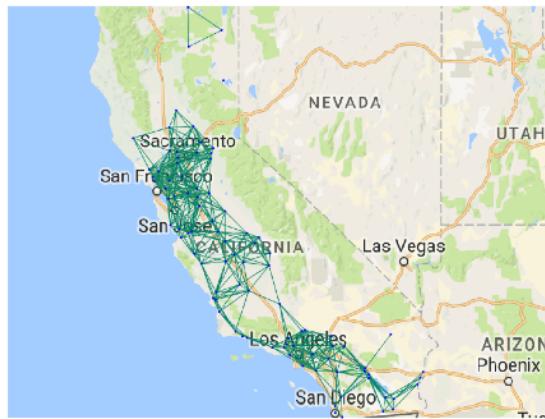
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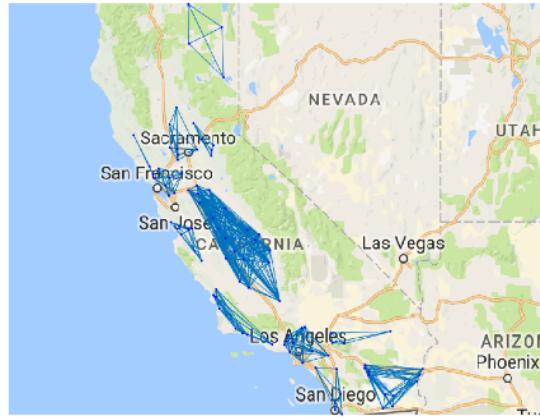


- The graph might (often) not be known a priori
- It becomes important to infer the proper structure

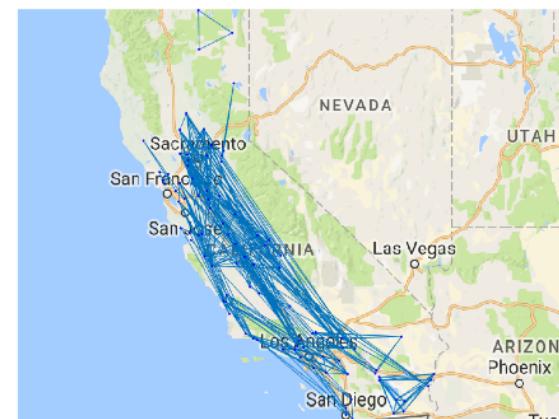
A simple example



Distance based

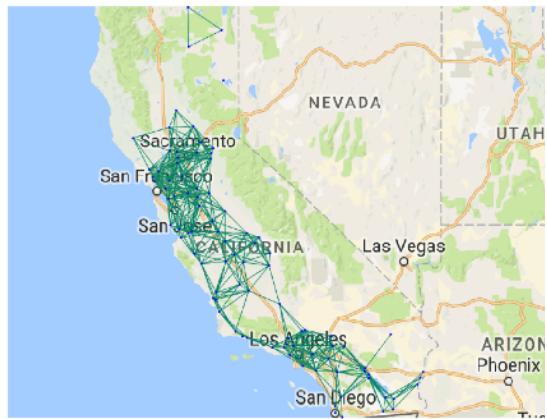


Region based

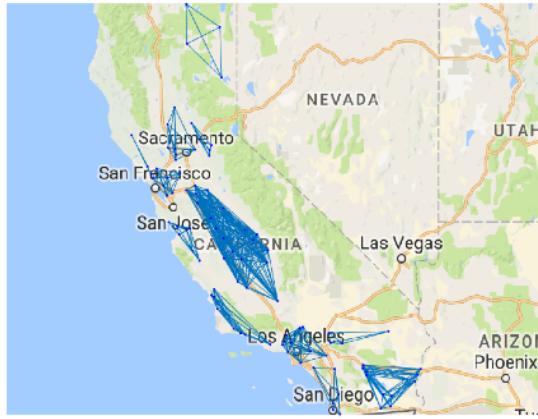


Evapotranspiration zone based

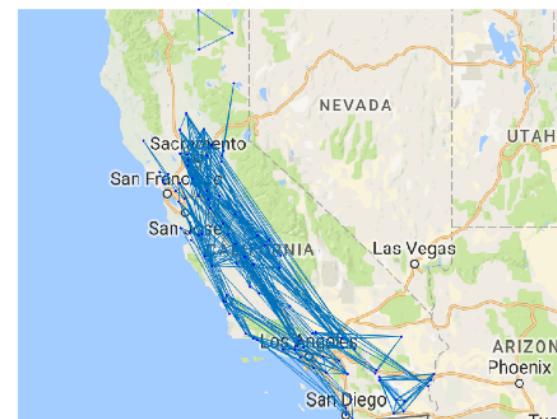
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Distance based



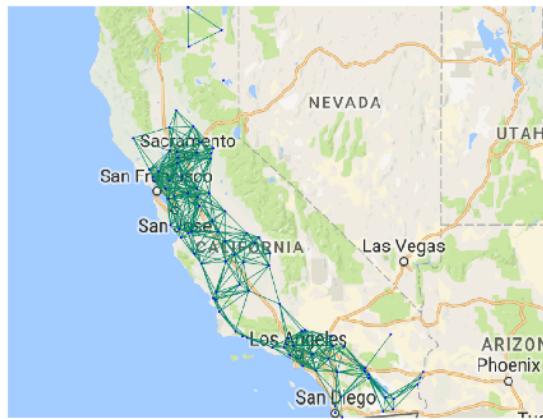
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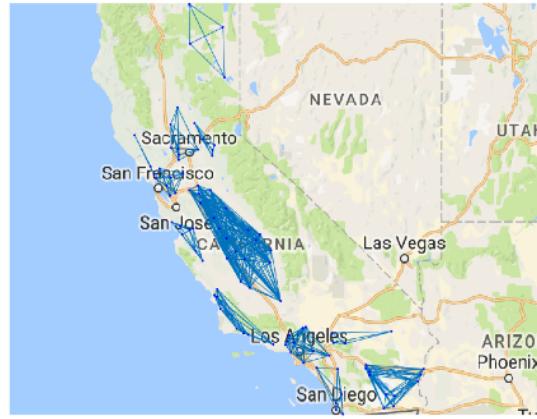
Evapotranspiration zone based

- What is the structure of my data?

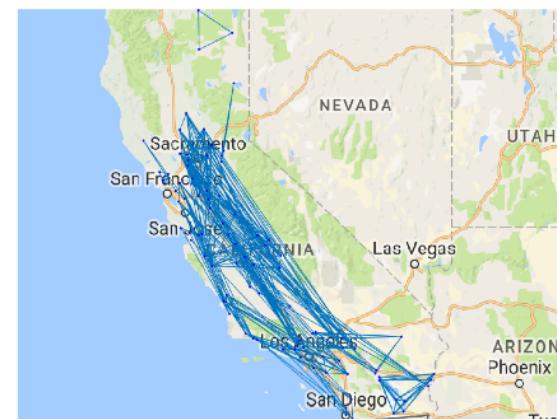
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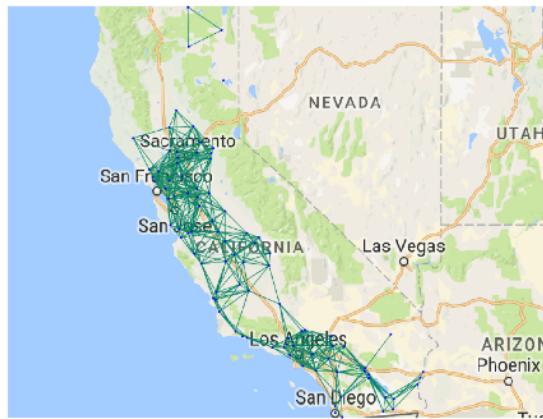
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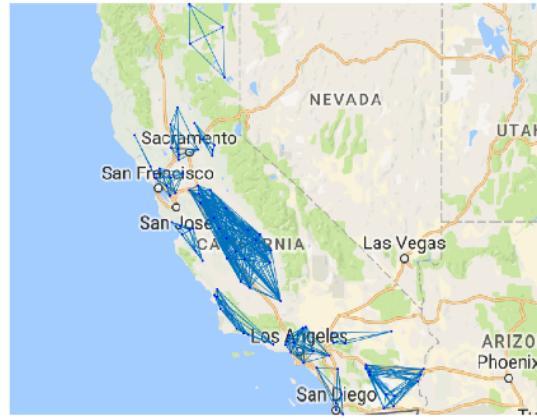
Evapotranspiration zone based

- What is the structure of my data?
- Can we use observations (e.g., temperature, humidity) to infer the right graph?

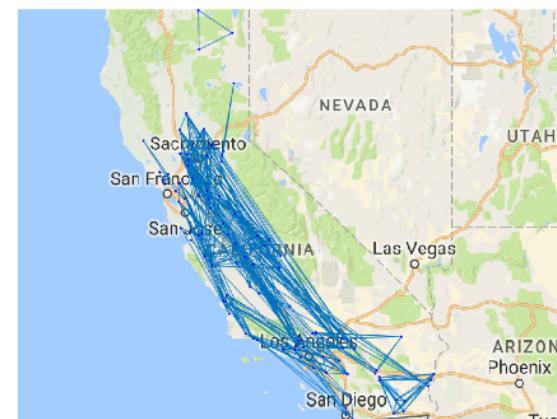
A simple example



Distance based



Region based

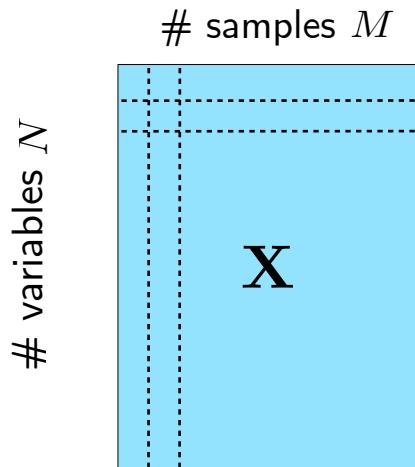


Evapotranspiration zone based

- What is the structure of my data?
- Can we use observations (e.g., temperature, humidity) to infer the right graph?
- What info about the data should the ‘optimal’ graph reveal?

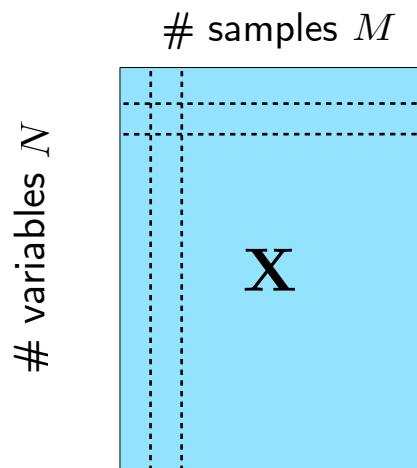
The topology inference problem

- **Different terminologies** in the literature:
 - covariance estimation
 - learning graphical models
 - network inference/graph learning
 - ...



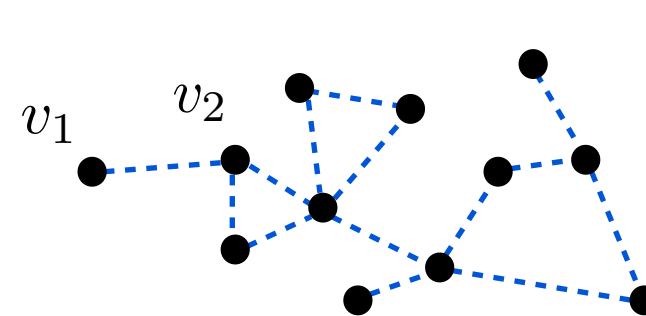
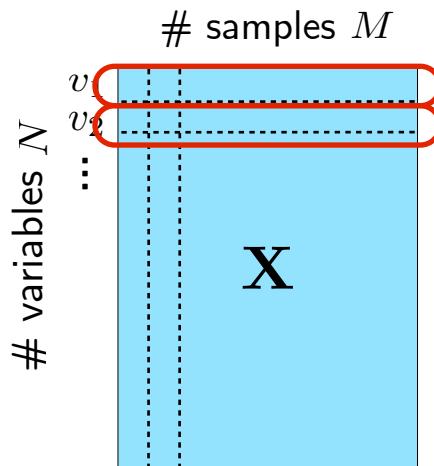
The topology inference problem

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- **Common goal:** Discover structure in the data by building a measure of relations between variables



The topology inference problem

- **Different terminologies** in the literature:
 - covariance estimation
 - learning graphical models
 - network inference/graph learning
 - ...
- **Common goal:** Discover structure in the data by building a measure of relations between variables



How do we build or learn a graph?

Topology inference methods

- **Model-free:**
 - do not assume any mechanism to generate the data
 - usually use statistical measures
- **Model-based:**
 - assume a mathematical model to generate the data/ signals
 - determine the model parameters to fit observed data

Model-free methods

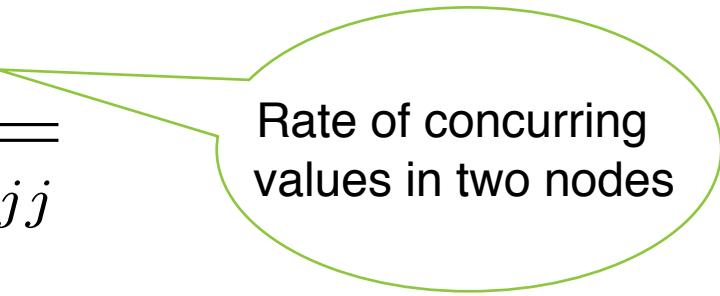
- **Sample correlation/Pearson correlation:**

$$\rho_{ij} = \frac{\sum_{ij}}{\sqrt{\sum_{ii}\sum_{jj}}}$$

Rate of concurring
values in two nodes

Model-free methods

- **Sample correlation/Pearson correlation:**

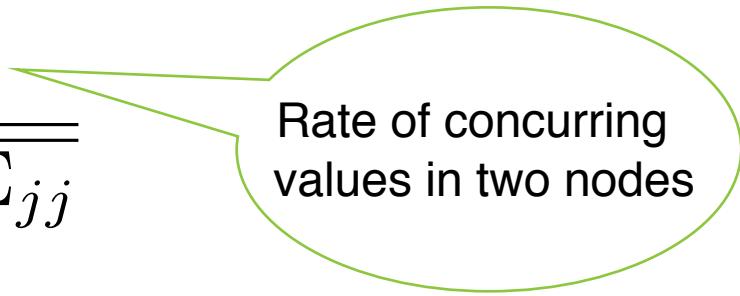
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Rate of concurring values in two nodes

- **K-NN graph:** Connect each node to its K nearest neighbors

Model-free methods

- **Sample correlation/Pearson correlation:**

$$\rho_{ij} = \frac{\sum_{ij}}{\sqrt{\sum_{ii}\sum_{jj}}}$$


Rate of concurring values in two nodes

- **K-NN graph:** Connect each node to its K nearest neighbors
- **Kernel-based graph:** Define a similarity measure based on a graph kernel (e.g., Gaussian)

$$W_{i,j} = \begin{cases} \exp\left(-\frac{[dist(i,j)]^2}{2\theta^2}\right), & \text{if } dist(i,j) \leq \kappa \\ 0, & \text{otherwise.} \end{cases}$$

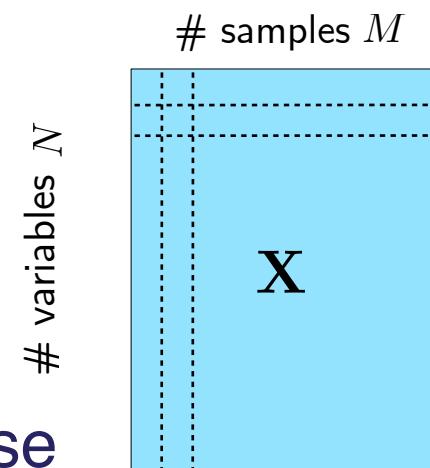
Model-free methods

- ✓ Computationally simple
- ✓ Intuitive
- Usually requires the definition of a good distance measure
- Need for parameter tuning
- Address pre/post-processing separately from connectivity inference
- Sensitive to noise

Model-based: Formal definition

- **Given:**

- M observations on N variables
- some prior knowledge (e.g., distribution, data model, etc) about the data



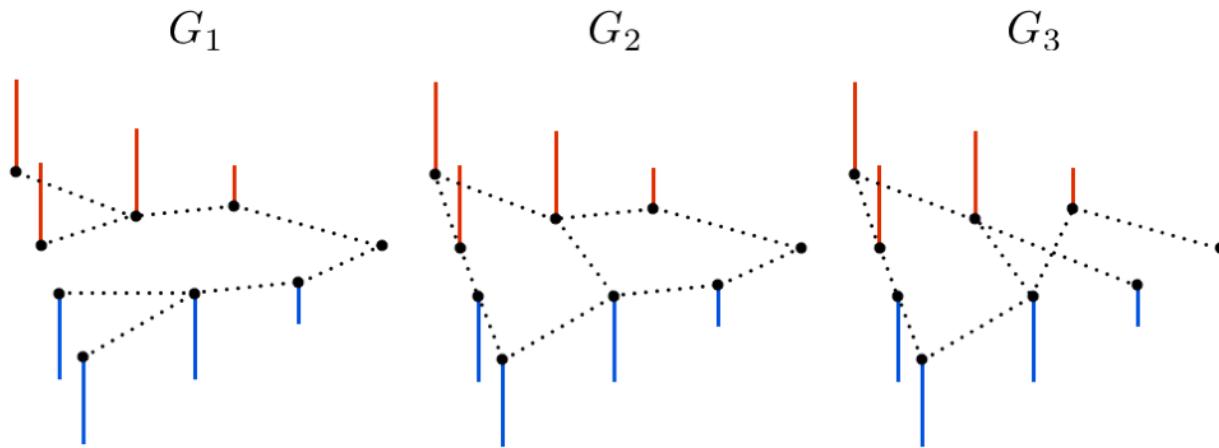
- **Goal:**

- Build or infer relationships between these variables that take the form of a graph

$$X = \mathcal{F}(G)$$

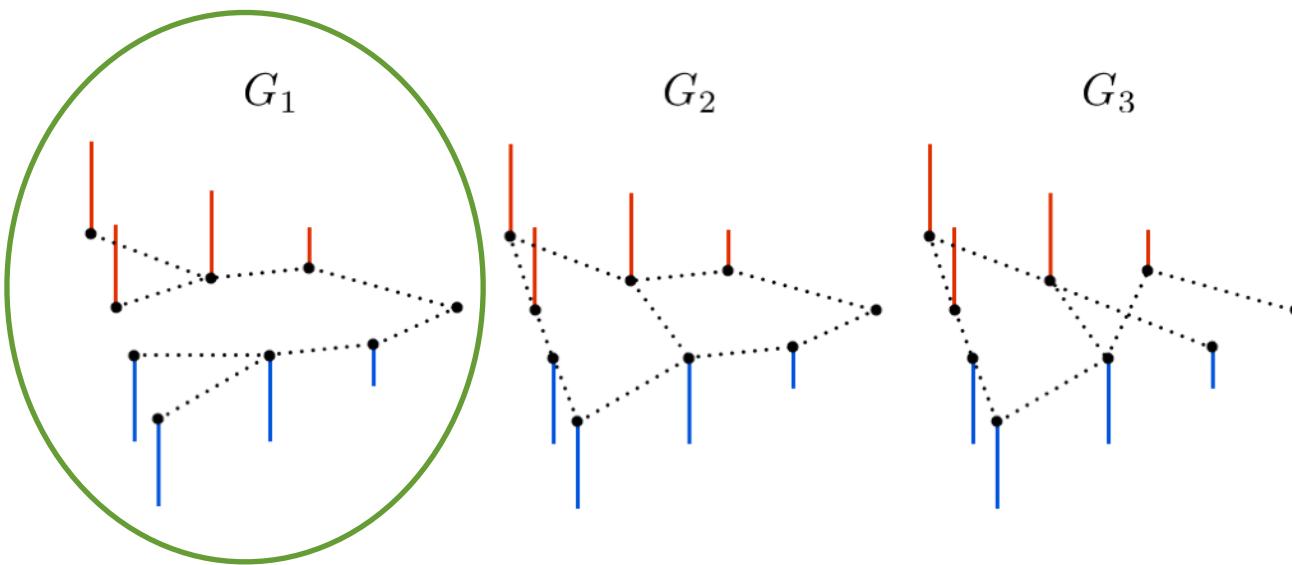
Model-based methods

- ✓ Easier to incorporate priors
- ✓ More robust to noise



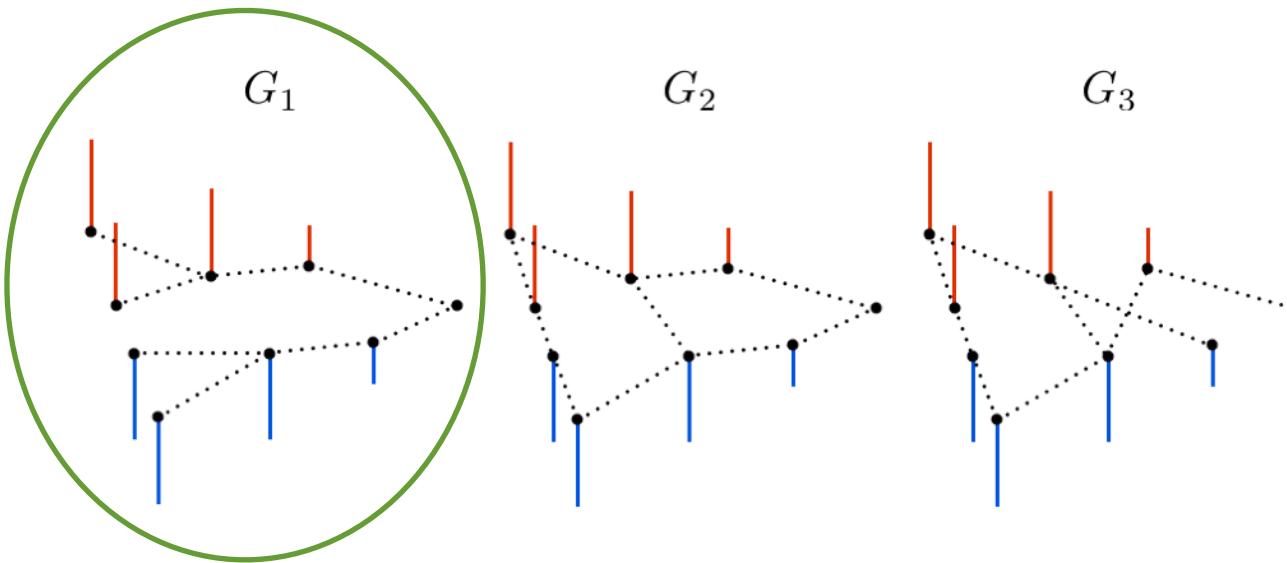
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Model-based methods

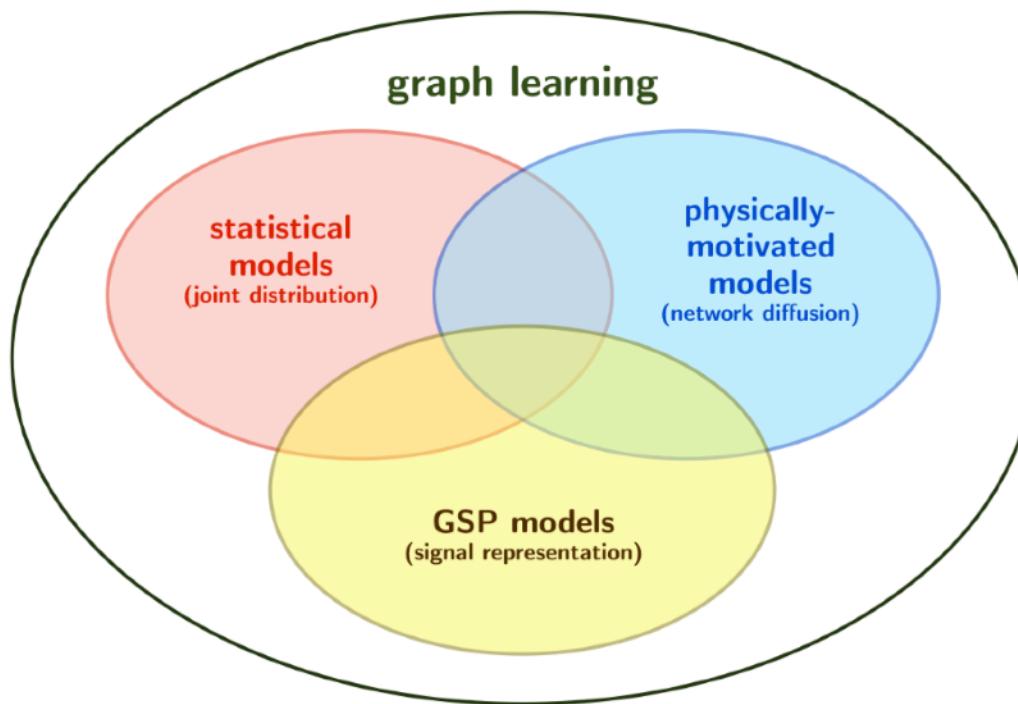
- ✓ Easier to incorporate priors
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- Scalability issues: The solution of a complex optimization problem is usually required

Model-based methods in a nutshell

- Different approaches...



- ... with however some similar assumptions

Outline

- A (partial) historical overview of model-based methods
- A graph signal processing perspective
 - A quick reminder of GSP
 - GSP for topology inference
- Applications/Concluding remarks

Outline

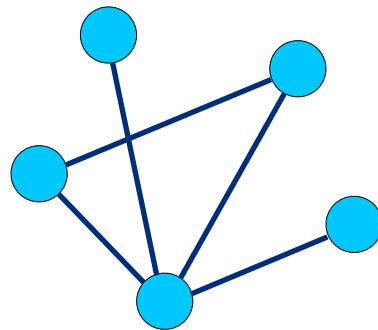
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Historical overview

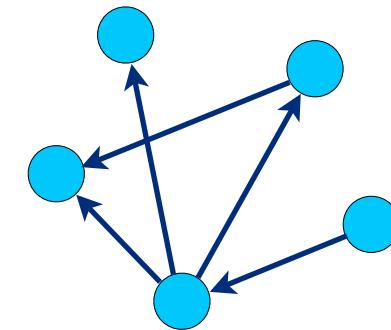
- Learning **graphical models**: probabilistic models for which the graph represent the conditional dependence between variables

Historical overview

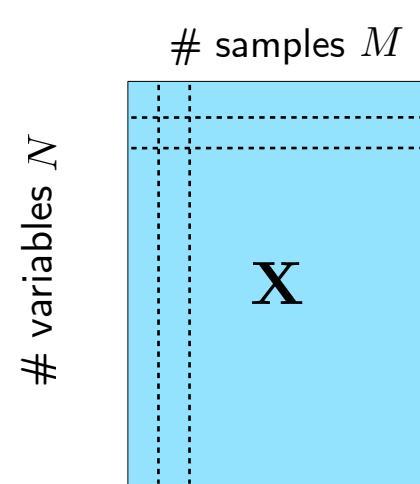
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Undirected graphical models:
Markov random fields (MRF)

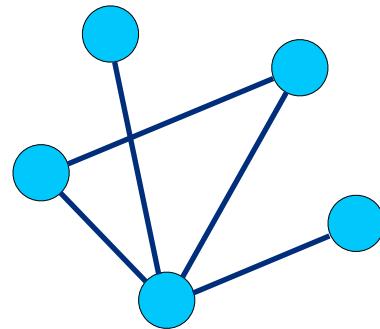


Directed graphical models:
Bayesian networks (BN)

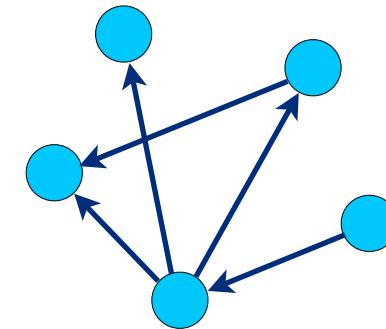


Historical overview

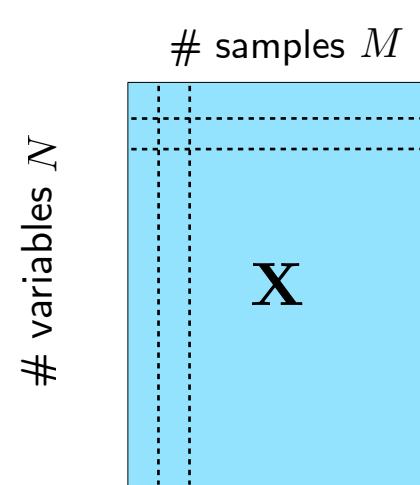
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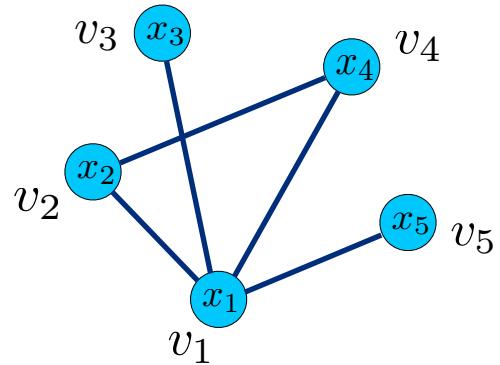


Directed graphical models:
Bayesian networks (BN)



Historical overview

- Learning pairwise MRF

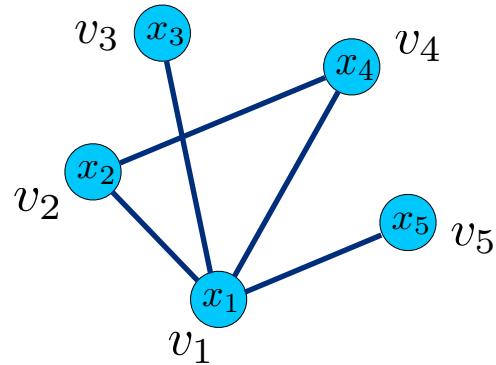


Historical overview

- Learning pairwise MRF

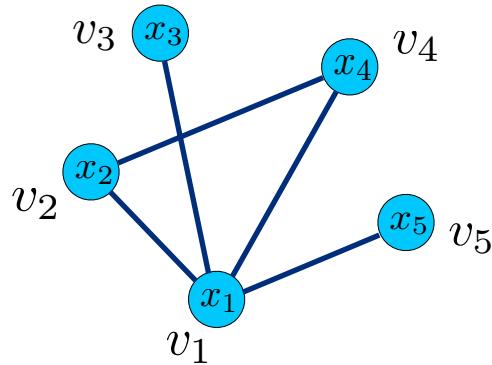
Conditional independence:

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



Historical overview

- Learning pairwise MRF



Conditional independence:

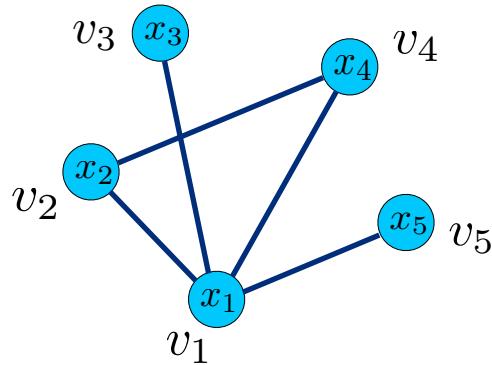
$$(i, j) \notin E \Leftrightarrow x_i \perp x_j \mid \mathbf{x} \setminus \{x_i, x_j\}$$

Probability parametrized by the precision matrix (inverse covariance) Θ :

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

Historical overview

- Learning pairwise MRF



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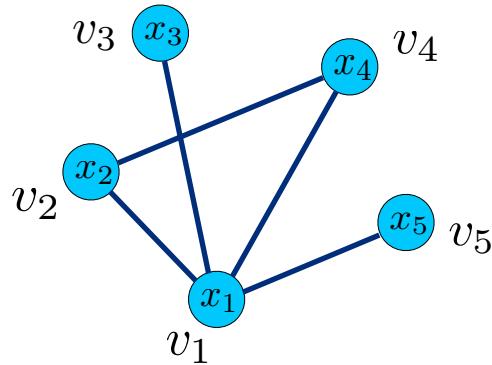
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Gaussian MRF with precision Θ :

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

Historical overview

- Learning pairwise MRF



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Learning a sparse Θ :

- interactions are mostly local
- computationally more tractable

Historical overview

*covariance
selection*

Dempster



1972

Prune the smallest elements in precision (inverse covariance) matrix

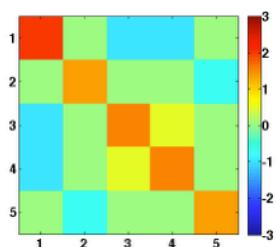
Historical overview

covariance selection

Dempster

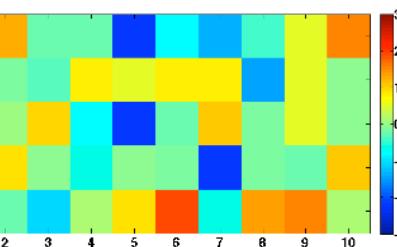
1972

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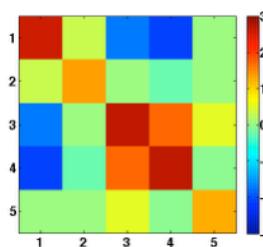
Θ

ground-truth
precision



$X \sim \mathcal{N}(0, \Theta)$

data matrix



S^{-1}

inverse of
sample covariance

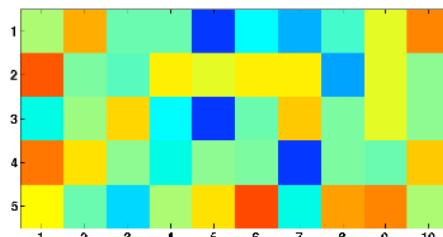
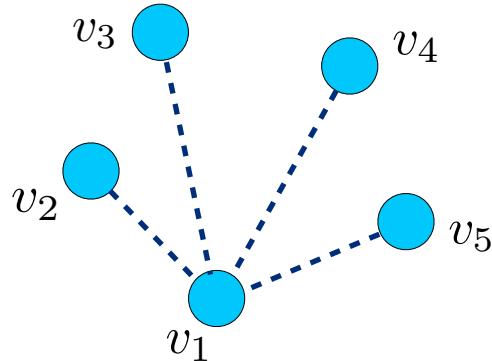
Historical overview

covariance selection
Dempster

ℓ_1 -regularized neighbourhood regression
Meinshausen & Bühlmann



Learning a graph = learning neighbourhood of each node



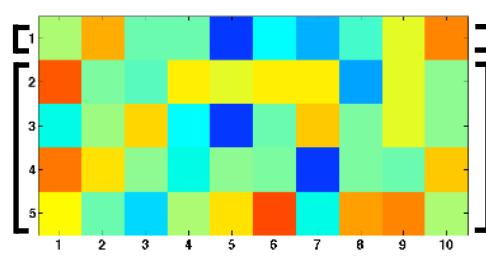
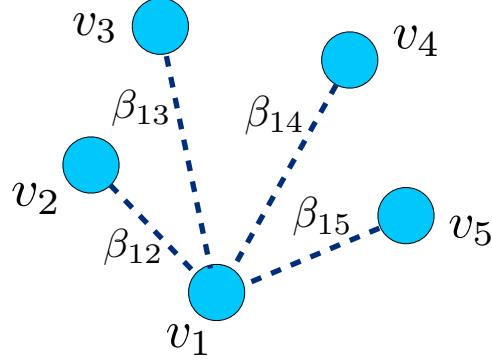
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$$\mathbf{X}_1^T$$

$$\mathbf{X}_{\setminus 1}^T$$

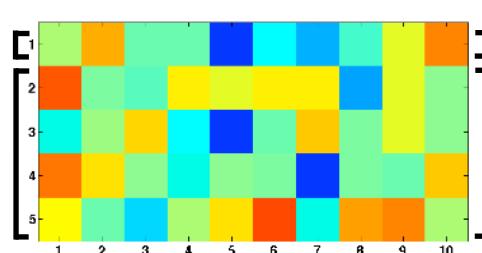
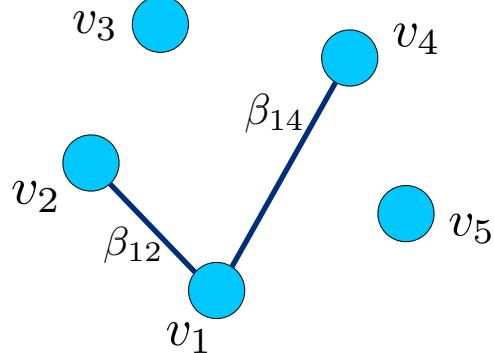
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covariance selection
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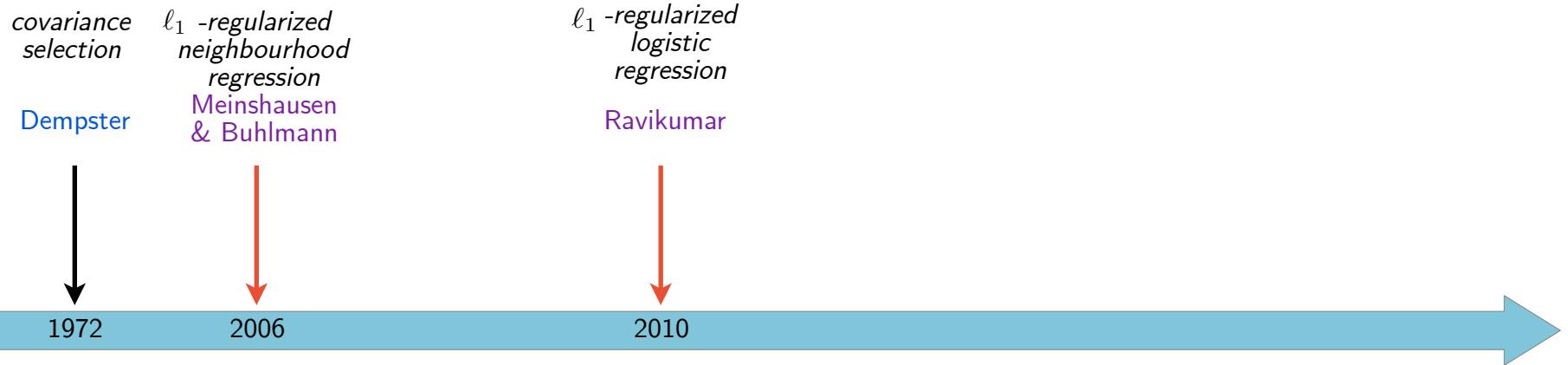


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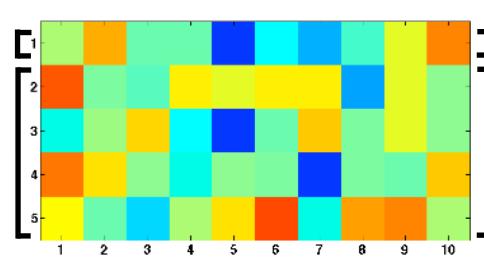
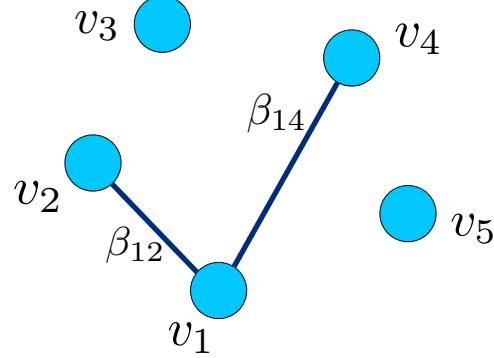
$$\mathbf{X}_{\setminus 1}^T$$

LASSO regression:
$$\min_{\boldsymbol{\beta}_1} \|\mathbf{X}_1 - \mathbf{X}_{\setminus 1}\boldsymbol{\beta}_1\|^2 + \lambda \|\boldsymbol{\beta}_1\|_1$$

Historical overview



Learning a graph = learning neighbourhood of each node



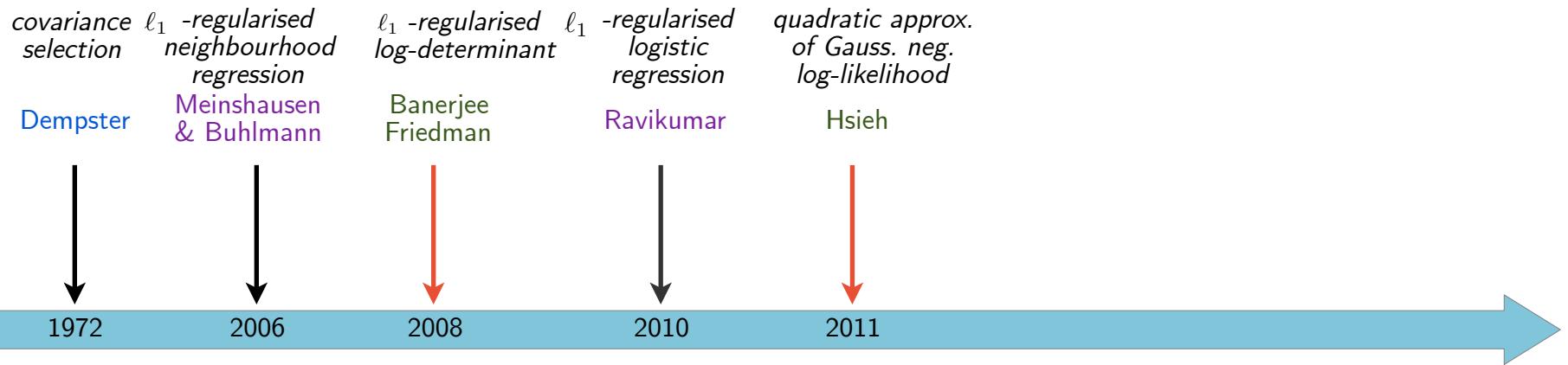
$$\mathbf{X}_1^T$$

$$\mathbf{X}_{\setminus 1}^T$$

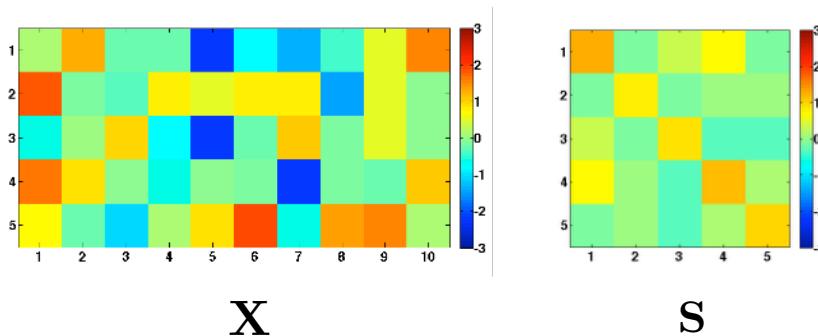
LASSO regression:
$$\min_{\boldsymbol{\beta}_1} \|\mathbf{X}_1 - \mathbf{X}_{\setminus 1}\boldsymbol{\beta}_1\|^2 + \lambda \|\boldsymbol{\beta}_1\|_1$$

Logistic regression for discrete variables

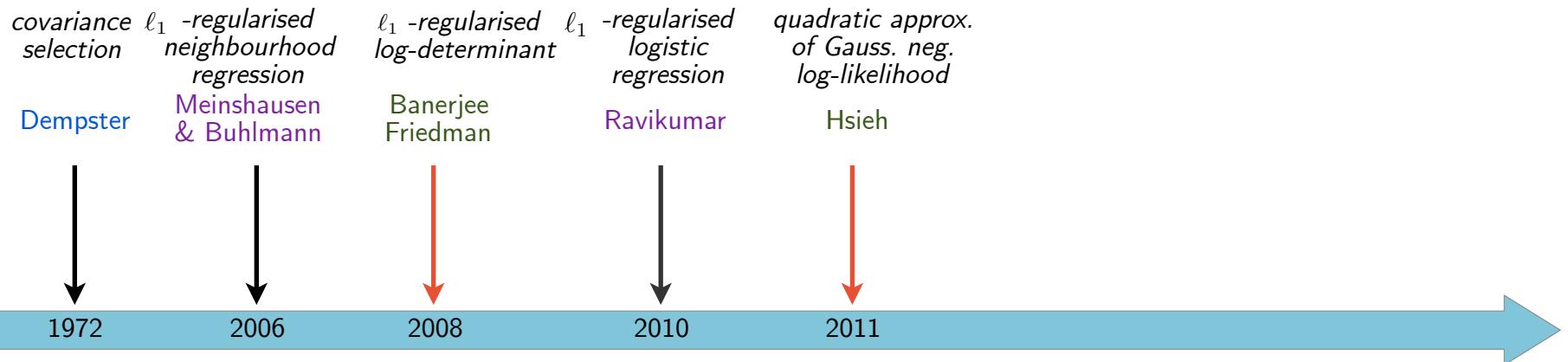
Historical overview



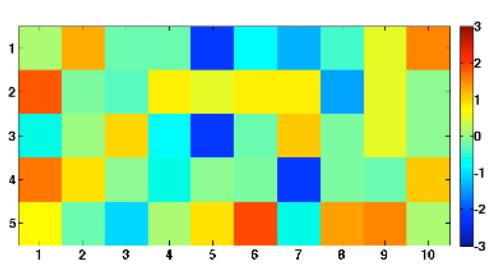
Estimation of sparse precision matrix



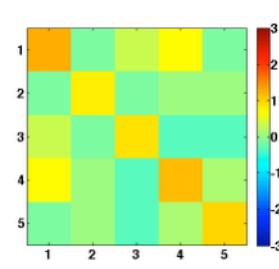
Historical overview



Estimation of sparse precision matrix



\mathbf{X}

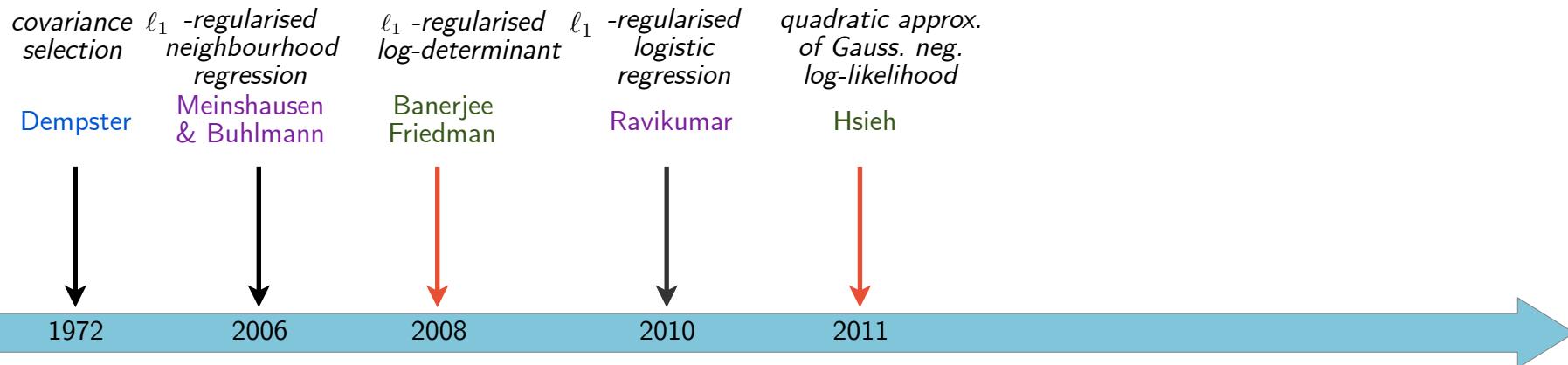


\mathbf{S}

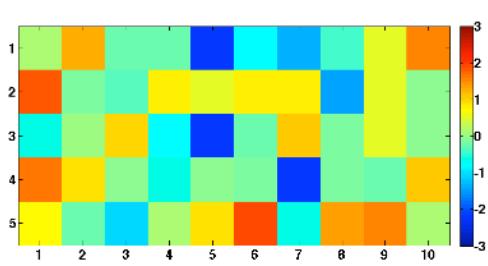
graphical LASSO maximizes likelihood of precision matrix Θ :

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

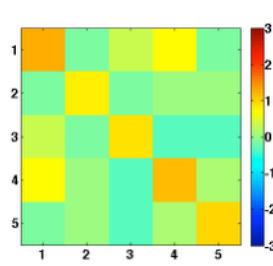
Historical overview



Estimation of sparse precision matrix



X



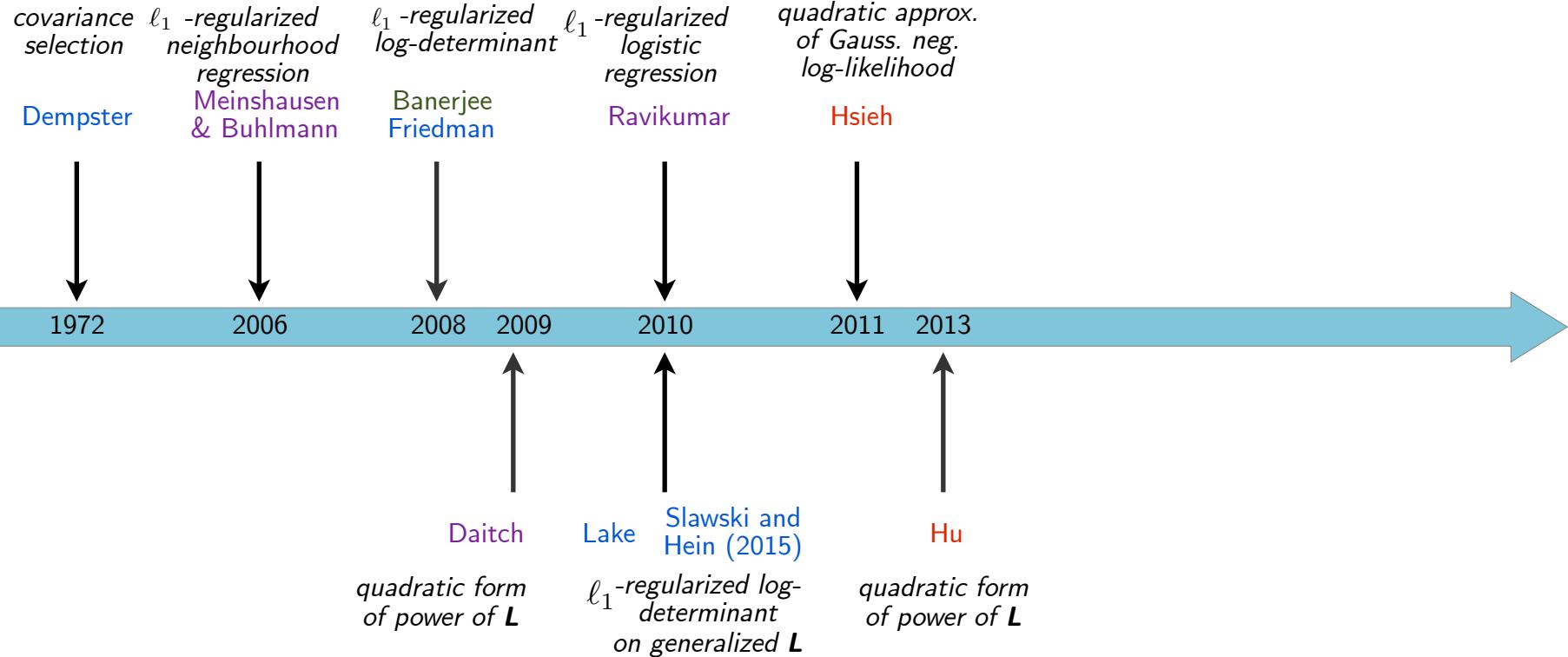
S

graphical LASSO maximizes likelihood of precision matrix Θ :

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

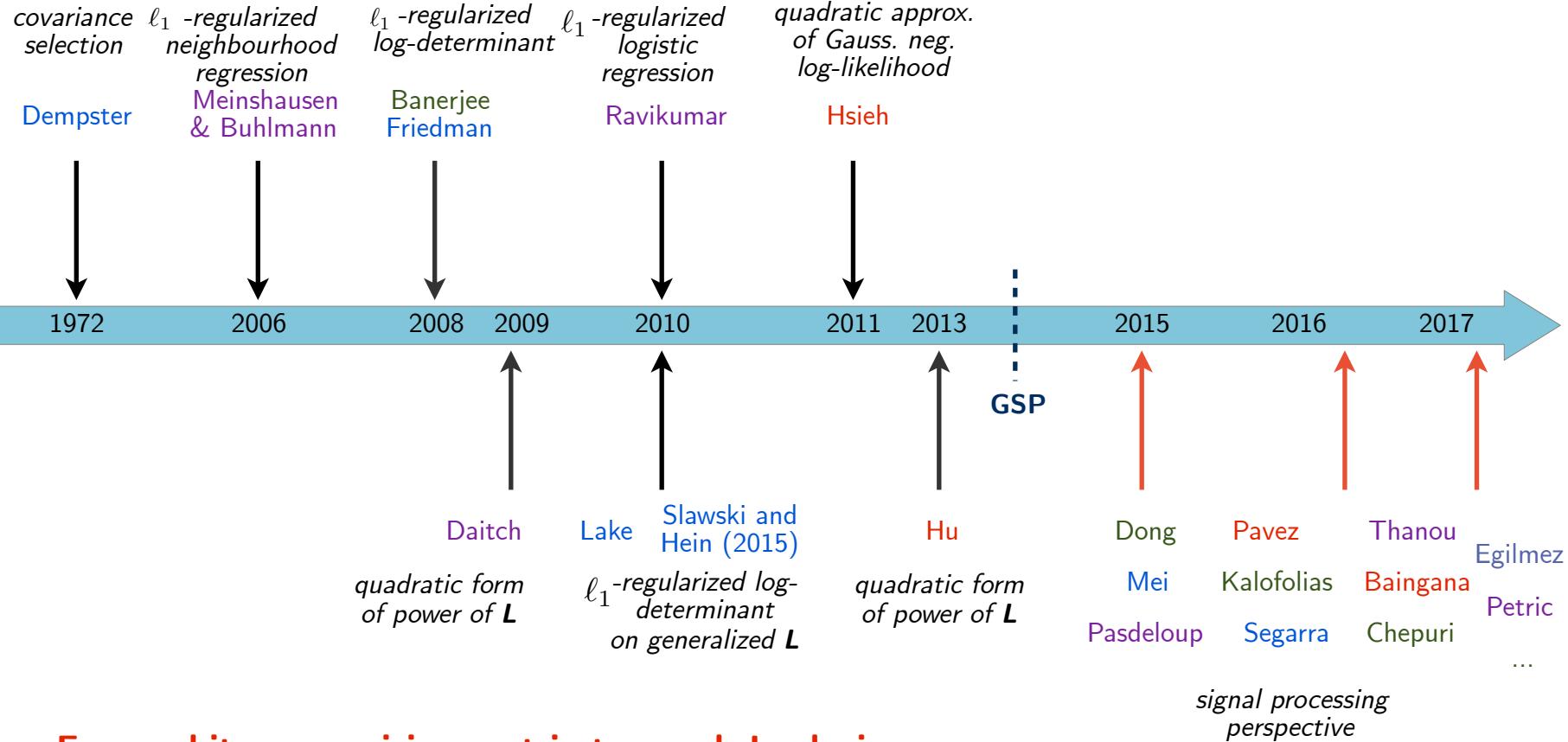
log-likelihood function

Historical overview



From arbitrary precision matrix to graph Laplacian

Historical overview



From arbitrary precision matrix to graph Laplacian

Common setting in graph signal processing

A signal processing approach?

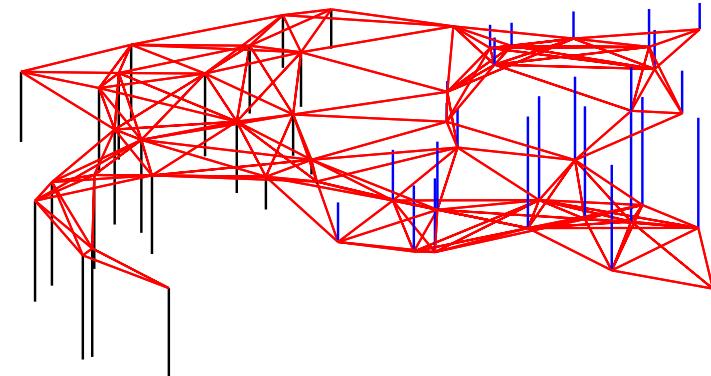
- Existing approaches have limitations
 - Simple correlation/similarity functions are simplistic
 - There is no strong emphasis on signal/graph interaction with spectral/frequency domain interpretation

Outline

- A partial historical overview
- **A graph signal processing perspective**
 - **A quick reminder of GSP**
 - **GSP for topology inference**
- Applications/Concluding remarks

Graphs and signals on graphs

- **Graph:** A mathematical tool $G = (\mathcal{V}, \mathcal{E}, W)$ for modelling the irregular domain
 - directed/**undirected**
 - **weighted**/unweighted
- Connectivity pattern captured by:
 - Adjacency A or weight matrix W (positive weights)
 - Laplacian matrix L
- **Graph signal:** A function $x : \mathcal{V} \rightarrow \mathbb{R}$ that assigns real values to each vertex of the graph



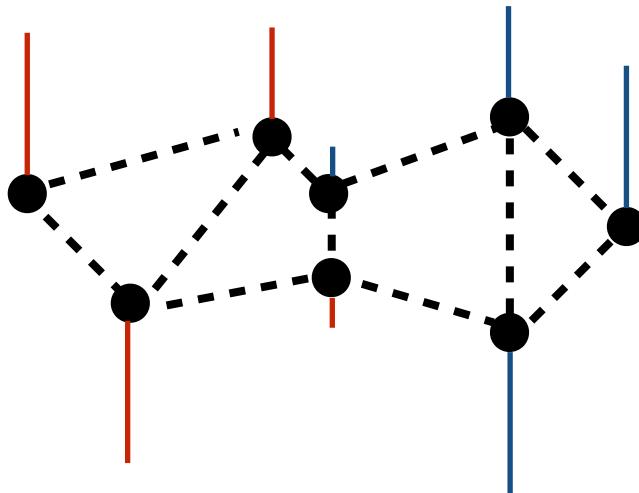
The graph Laplacian operator

- It is defined as $L = D - W$
 - Complete set of eigenvectors $\chi = [\chi_0, \chi_1, \dots, \chi_{N-1}]$
 - Non-negative eigenvalues $0 = \lambda_0 \leq \dots \leq \lambda_{N-1}$
- Defines global smoothness on graphs

$$x^T L x = \sum_{m \in \mathcal{V}} \sum_{n \in \mathcal{N}_m} W_{m,n} [x(m) - x(n)]^2$$

The graph Laplacian operator

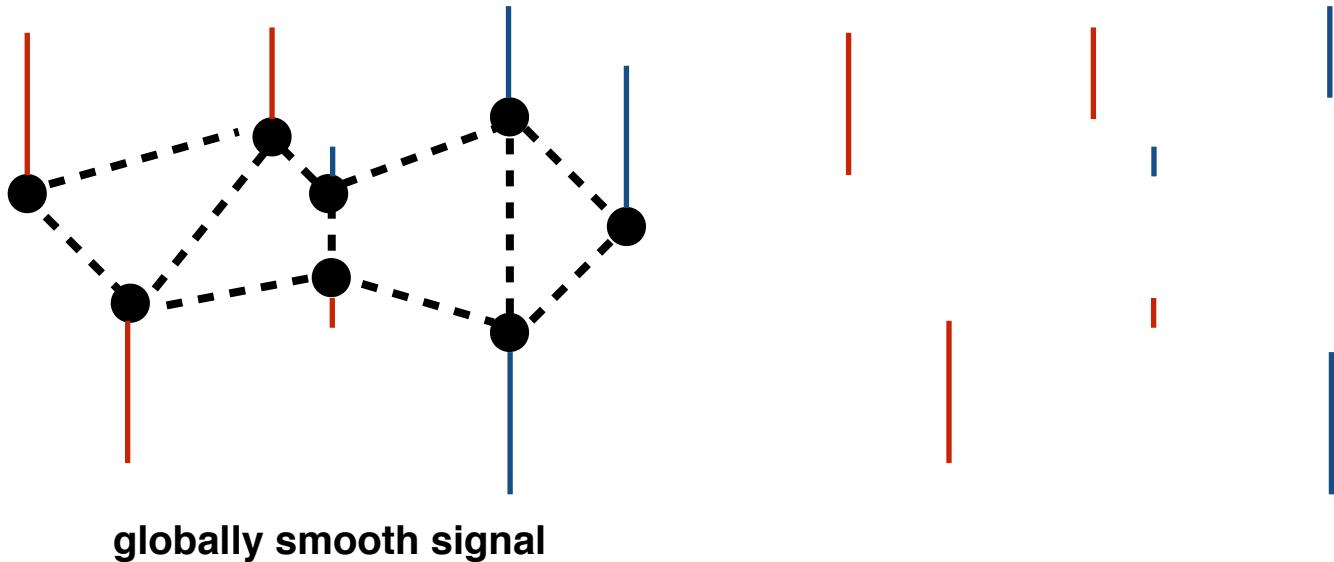
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globally smooth signal

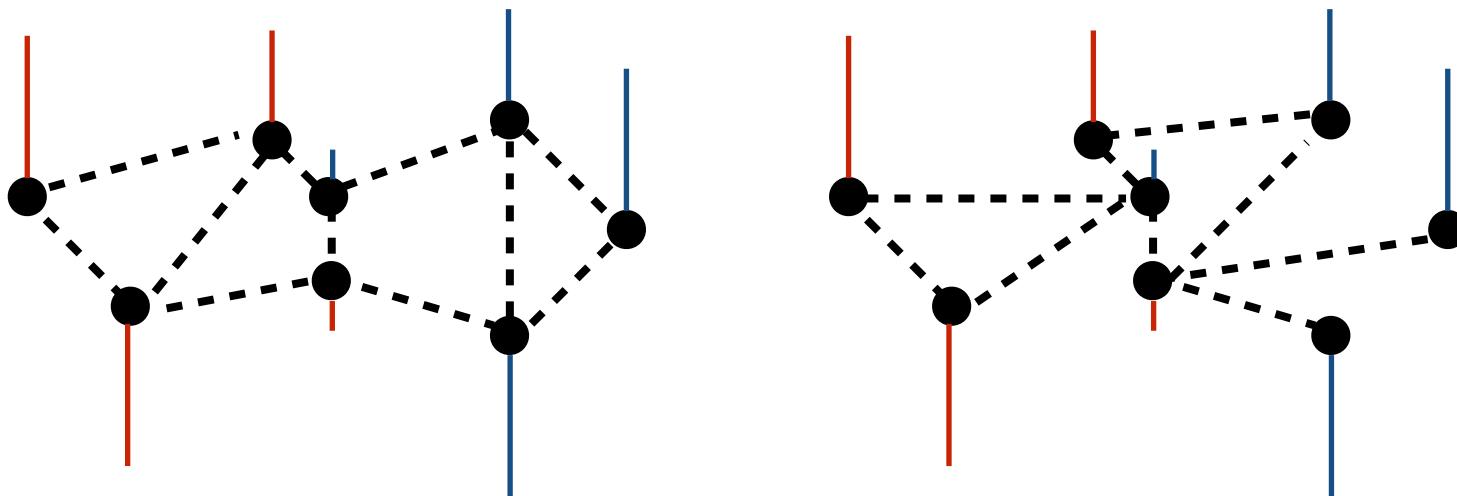
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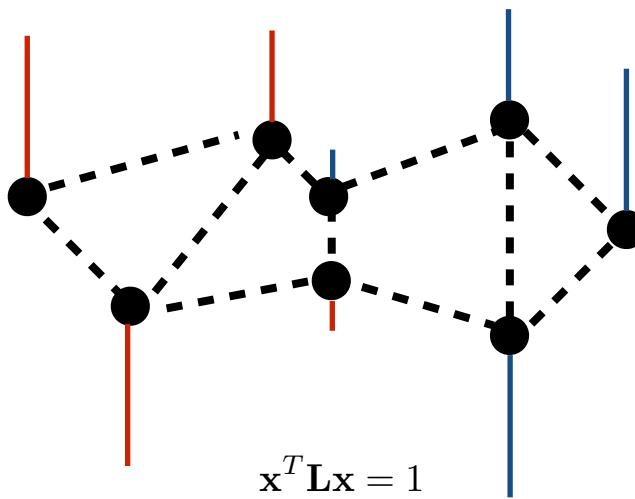
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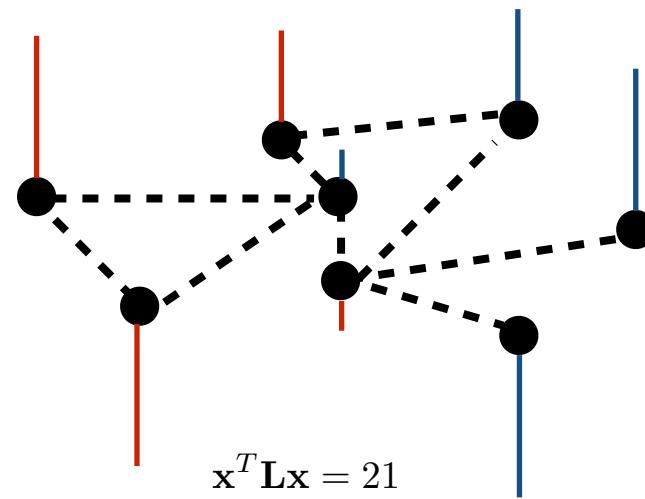


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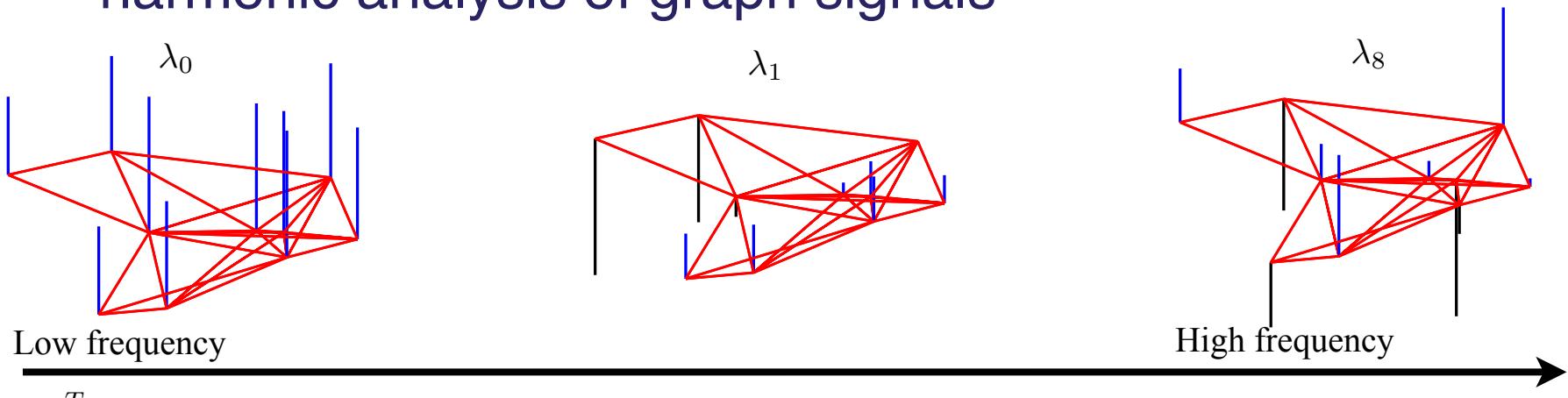
globally smooth signal



high frequency signal

The graph Fourier transform

- The eigenvectors of the Laplacian provide an harmonic analysis of graph signals



$$\mathbf{GFT} \quad \hat{x}(\lambda_\ell) = \langle x, \chi_\ell \rangle = \sum_{n=1}^N x(n) \chi_\ell(n)$$

$$\text{IGFT} \quad x(n) = \sum_{\ell=0} \hat{x}(\lambda_\ell) \chi_\ell(n)$$

Filtering on graphs

- Filtering in the spectral domain with a transfer function $\hat{g}(\cdot)$

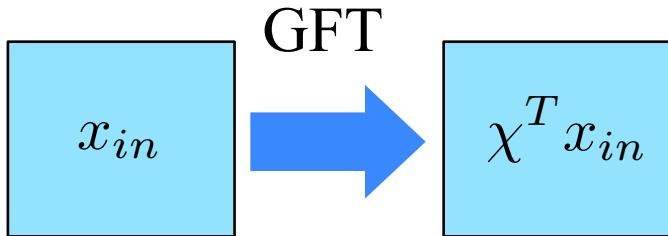
Filtering on graphs

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x_{in}

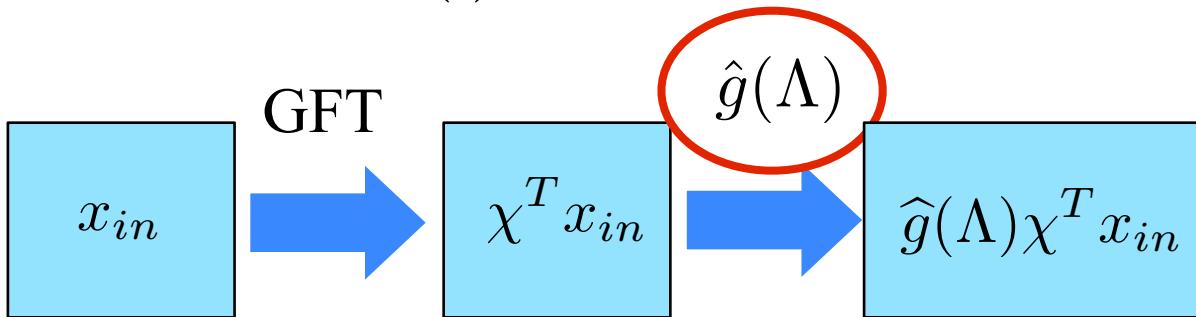
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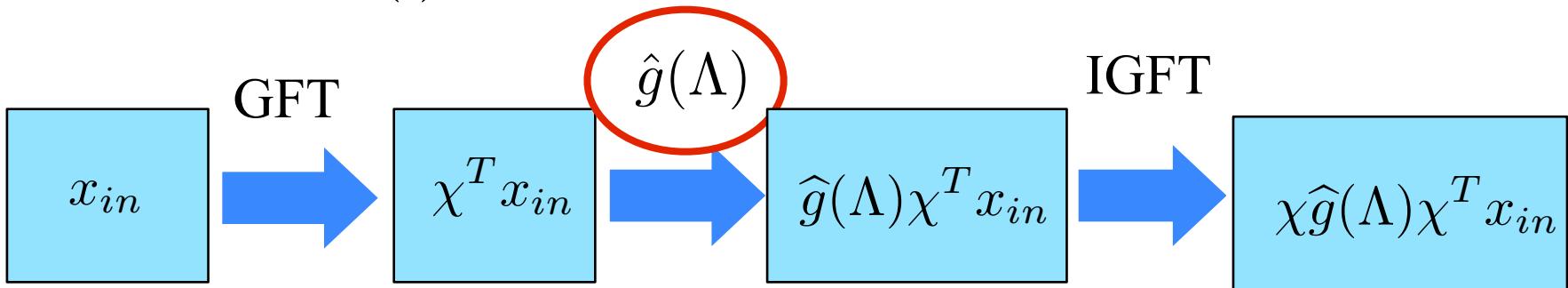
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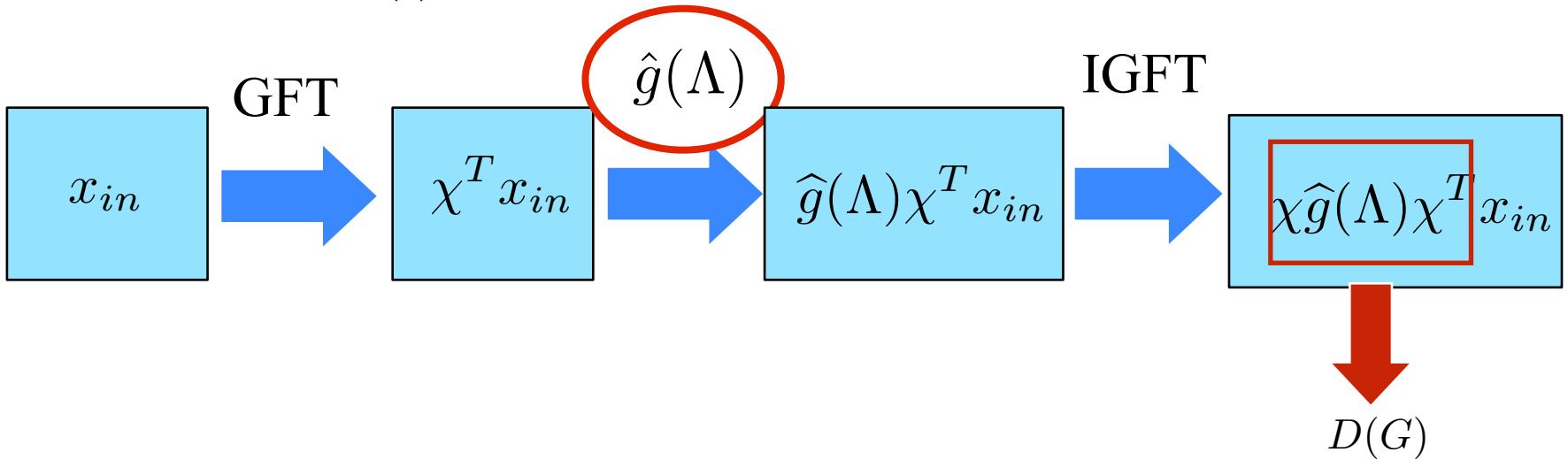
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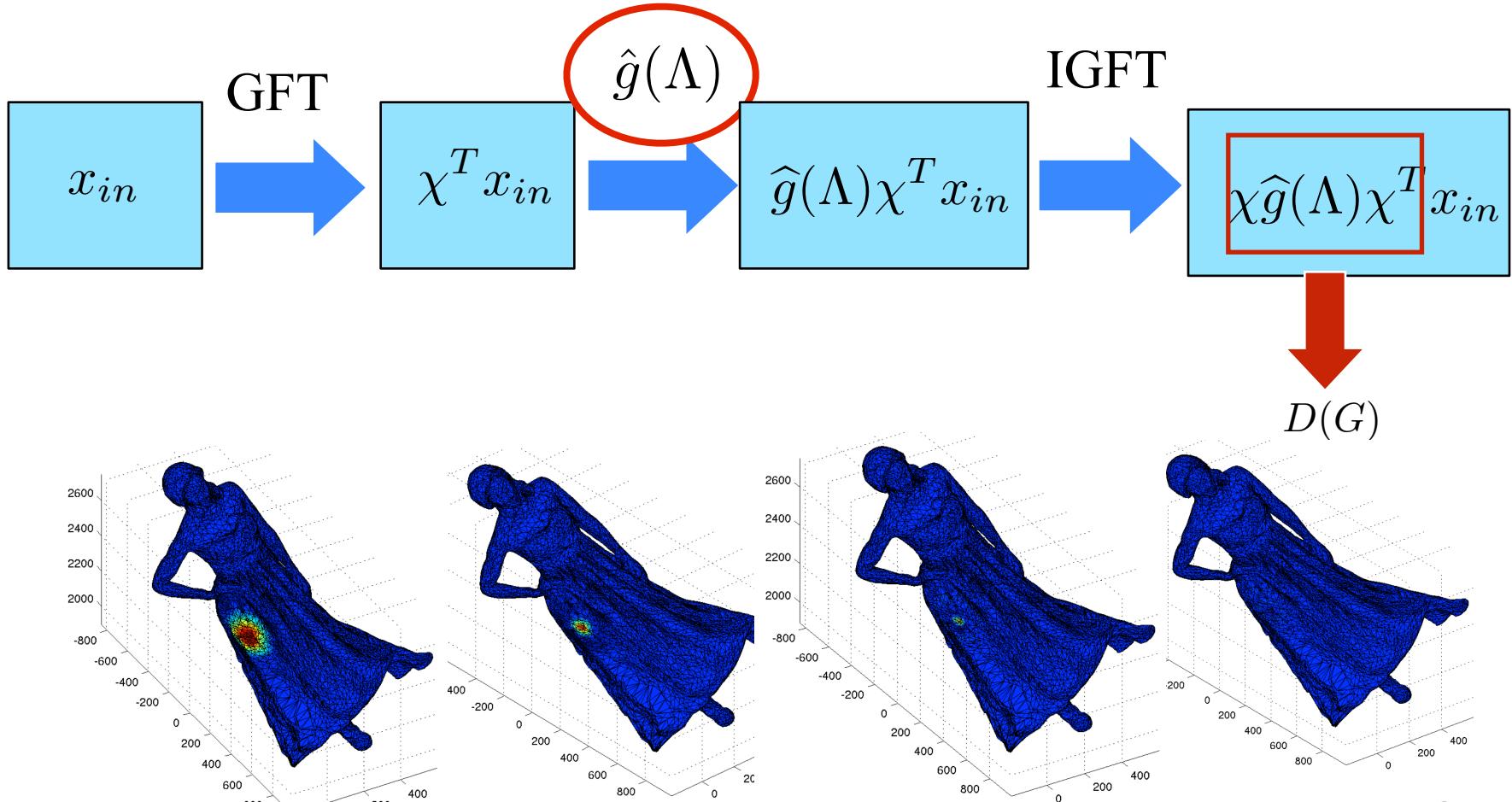
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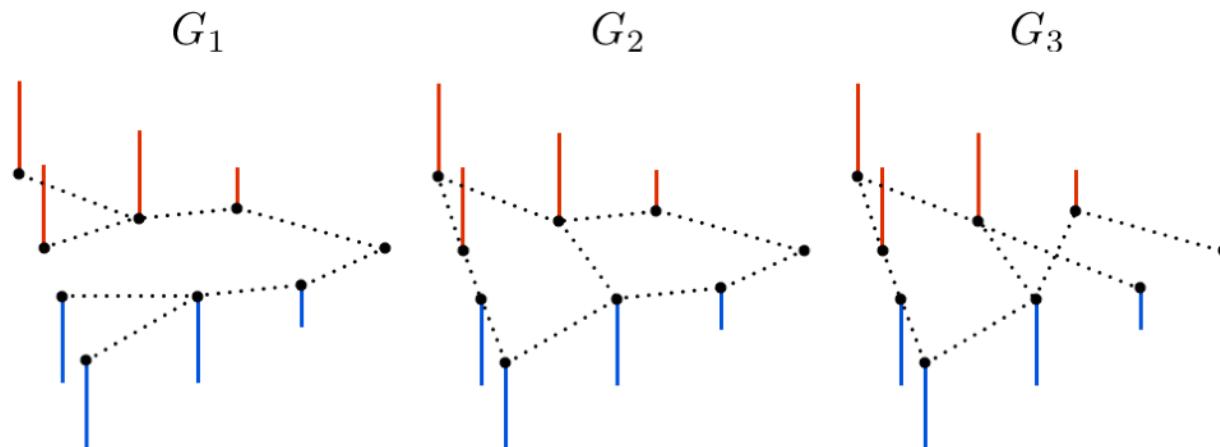


Topology inference revisited: A GSP perspective

- Define graph signal representation models
- Strong emphasis on signal/graph interaction with spectral/frequency-domain interpretation

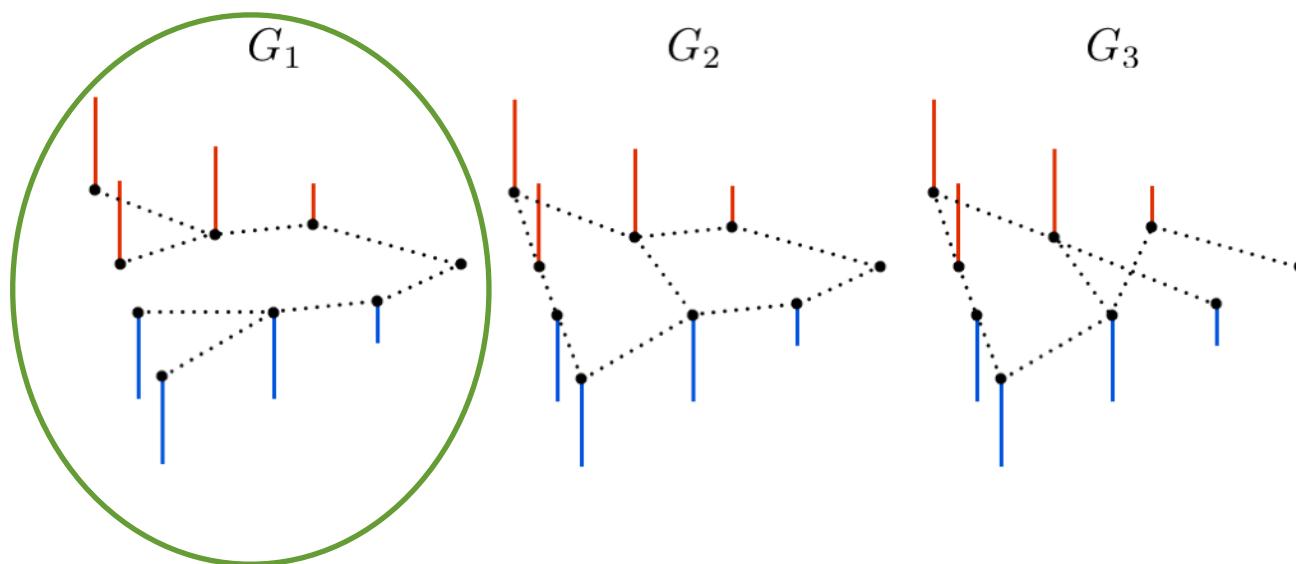
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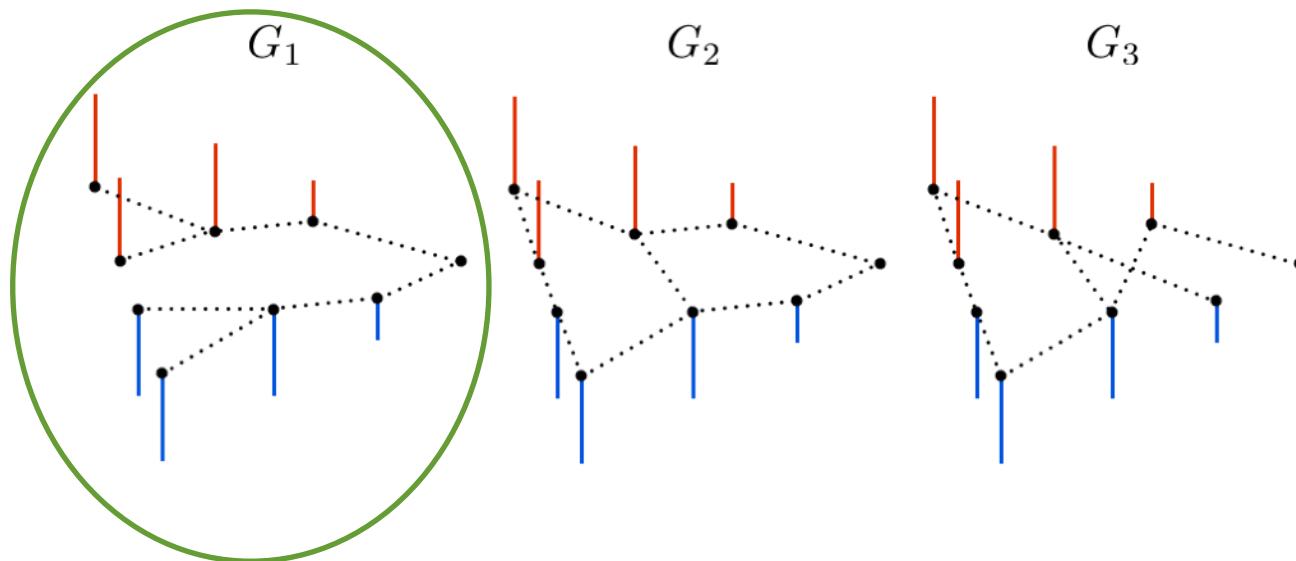
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Topology inference revisited: A GSP perspective

- Define graph signal representation models
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**Can we exploit the interplay between graphs and signals
on graphs to discover the topology?**

Graph signal representations

- Signal processing is about $Dc \approx x$

$$\begin{matrix} \text{D} & \times & \text{c} & = & \text{x} \end{matrix}$$

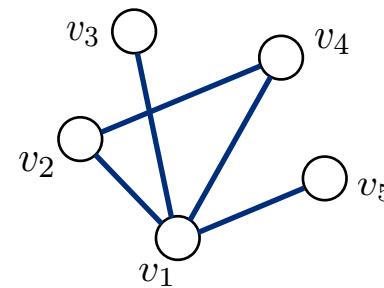
The diagram illustrates the multiplication of a 5x5 matrix \mathbf{D} (graph adjacency matrix) by a 5x1 vector \mathbf{c} (signal vector) to produce a 5x1 vector \mathbf{x} (transformed signal vector). The matrix \mathbf{D} is shown as a grid of colored squares, and the vectors \mathbf{c} and \mathbf{x} are shown as vertical stacks of colored squares. The multiplication is indicated by the symbol \times between \mathbf{D} and \mathbf{c} , and the result is indicated by the symbol $=$ followed by \mathbf{x} .

Graph signal representations

- Signal processing is about $Dc \approx x$
- Graph signal processing is about $D(G)c \approx x$

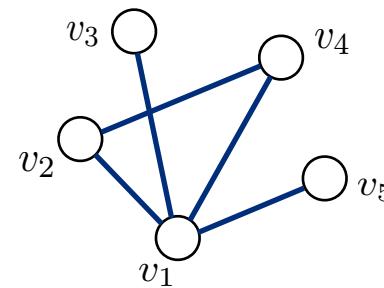
$$\begin{matrix} \text{D}(\mathcal{G}) & \times & \text{c} & = & \text{x} \\ \begin{matrix} \text{A 5x5 matrix with colored blocks:} \\ \text{Row 1: Blue, Yellow, Red, Yellow, Cyan} \\ \text{Row 2: Green, Yellow, Yellow, Green, Red} \\ \text{Row 3: Orange, Yellow, Yellow, Orange, Yellow} \\ \text{Row 4: Green, Cyan, Green, Yellow, Orange} \\ \text{Row 5: Orange, Yellow, Red, Cyan, Cyan} \end{matrix} & & \begin{matrix} \text{A 5x1 vector:} \\ \text{Row 1: Green} \\ \text{Row 2: Orange} \\ \text{Row 3: Blue} \\ \text{Row 4: Orange} \\ \text{Row 5: Red} \end{matrix} & & \begin{matrix} \text{A 5x1 vector:} \\ \text{Row 1: Orange} \\ \text{Row 2: Yellow} \\ \text{Row 3: Orange} \\ \text{Row 4: Red} \\ \text{Row 5: Blue} \end{matrix} \end{matrix}$$

\mathcal{G}



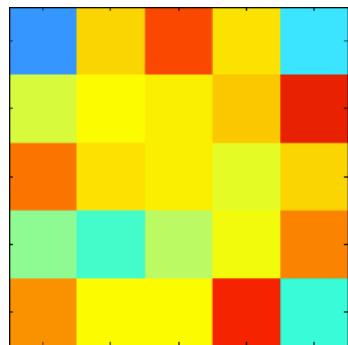
Graph signal representations

- Forward step: Given x, G , design D to study c

$$\mathbf{D}(\mathcal{G}) \times \mathbf{c} = \mathbf{x}$$


Graph signal representations

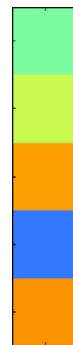
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$\mathbf{D}(\mathcal{G})$

Fourier/wavelet
atoms

\times



\mathbf{c}

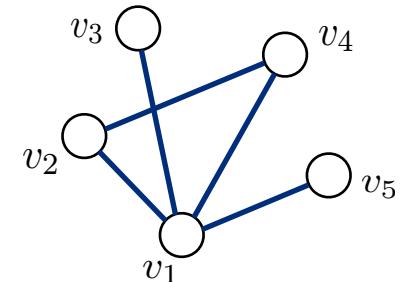
graph Fourier/
wavelet coefficient

$=$



\mathbf{x}

graph dictionary
coefficient



\mathcal{G}

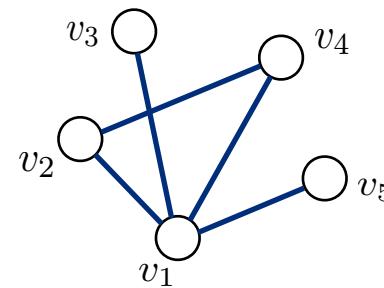
[Coifman06, Narang09, Hammond11, Shuman13, Sandryhaila13]

trained dictionary
atoms

[Zhang12, Thanou14]

Graph signal representations

- Forward step: Given x, G , design D to study c

$$\mathbf{D}(\mathcal{G}) \times \mathbf{c} = \mathbf{x}$$


Graph signal representations

- Forward step: Given x, G , design D to study c
- Backward (topology inference): Given x , design D, c to infer G

$$\begin{matrix} \text{D}(\mathcal{G}) & \times & \mathbf{c} & = & \mathbf{x} \\ \begin{matrix} \text{A 6x6 matrix with colored blocks: } \\ \text{Row 1: Blue, Yellow, Red, Yellow, Cyan, Light Blue} \\ \text{Row 2: Light Green, Yellow, Yellow, Light Green, Red, Orange} \\ \text{Row 3: Orange, Yellow, Yellow, Light Green, Cyan, Orange} \\ \text{Row 4: Light Green, Cyan, Light Green, Yellow, Orange, Orange} \\ \text{Row 5: Orange, Yellow, Yellow, Light Green, Red, Cyan} \\ \text{Row 6: Light Green, Yellow, Red, Cyan, Cyan, Light Blue} \end{matrix} & & \begin{matrix} \text{A 6x1 vector: } \\ \text{Row 1: Green} \\ \text{Row 2: Light Green} \\ \text{Row 3: Orange} \\ \text{Row 4: Blue} \\ \text{Row 5: Orange} \\ \text{Row 6: Orange} \end{matrix} & & \begin{matrix} \text{A 6x1 vector: } \\ \text{Row 1: Orange} \\ \text{Row 2: Yellow} \\ \text{Row 3: Orange} \\ \text{Row 4: Red} \\ \text{Row 5: Blue} \\ \text{Row 6: Cyan} \end{matrix} \end{matrix}$$

\mathcal{G}

Graph signal representations

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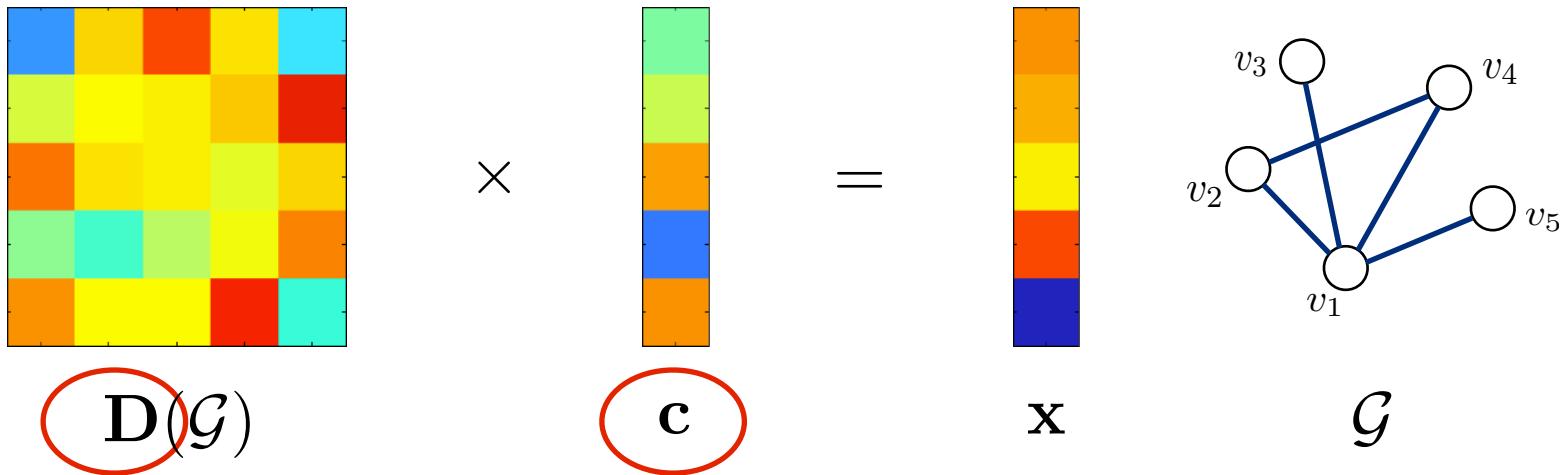
$$\begin{matrix} \text{D}(G) & \times & \mathbf{c} & = & \mathbf{x} \\ \text{---} & & \text{---} & & \text{---} \end{matrix}$$

The diagram illustrates the forward step of graph signal representation. It shows the multiplication of a graph operator matrix $D(G)$ (circled in red) and a signal vector c to produce a transformed signal vector x . The matrix $D(G)$ is a 6x6 grid with colored blocks representing different graph features. The vector c is a 6x1 column with colored segments. The resulting vector x is also a 6x1 column with colored segments. To the right, a graph G is shown with 5 nodes labeled v_1 through v_5 and various edges connecting them.

- The key is a signal/graph model behind \mathbf{D}
- Designed around graph operators (adjacency/Laplacian matrices, shift operators)

Graph signal representations

- Forward step: Given x, G , design D to study c
- Backward (topology inference): Given x , design D, c to infer G



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

Model 1: Global smoothness

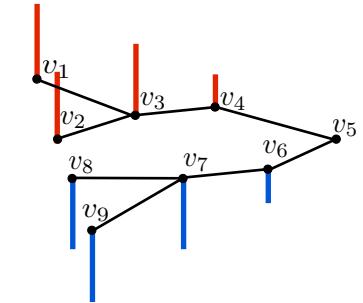
- Connected nodes on the graph have similar signal values
- Usually quantified by the Laplacian quadratic form:

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

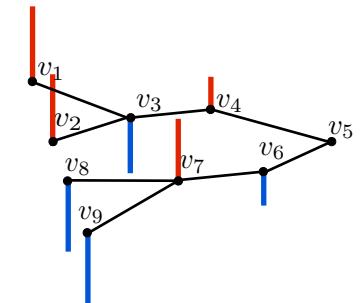
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$$\mathbf{x}^T \mathbf{L} \mathbf{x} = 1$$



$$\mathbf{x}^T \mathbf{L} \mathbf{x} = 21$$

Model 1: Global smoothness

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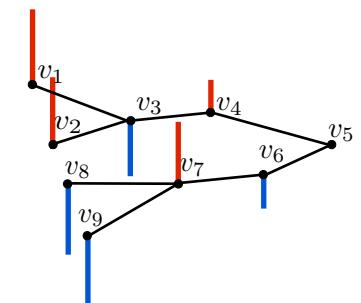
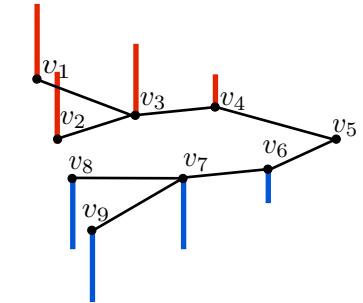
$$\mathbf{x}^T \mathbf{L} \mathbf{x} = \frac{1}{2} \sum_{i,j} \mathbf{W}_{ij} (\mathbf{x}(i) - \mathbf{x}(j))^2$$

Similar to previous approaches:

Lake (2010): $\max_{\Theta = \mathbf{L} + \frac{1}{\sigma^2} \mathbf{I}} \log \det \Theta - \frac{1}{M} \text{tr}(\mathbf{X} \mathbf{X}^T \Theta) - \rho \|\Theta\|_1$

Daitch (2009): $\min_{\mathbf{L}} \mathbf{X}^T \mathbf{L}^2 \mathbf{X}$

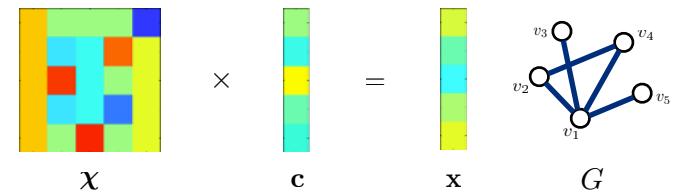
Hu (2013): $\min_{\mathbf{L}} \text{tr}(\mathbf{X}^T \mathbf{L}^s \mathbf{X}) - \beta \|\mathbf{W}\|_F$



Model 1: Global smoothness

- Dong et al (2015), Kalofolias (2016)

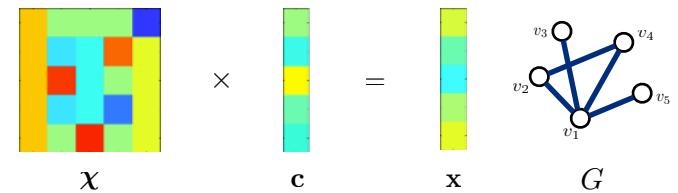
- $D(G) = \chi$ (eigenvector matrix of \mathbf{L})
- Gaussian assumption on \mathbf{c} : $\mathbf{c} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Lambda})$
- Gaussian Markov Random Field
 $x \sim \mathcal{N}(0, L^\dagger + \sigma_\epsilon^2 I)$



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- Maximum a posteriori (MAP) estimation of c leads to minimization of the Laplacian quadratic form:

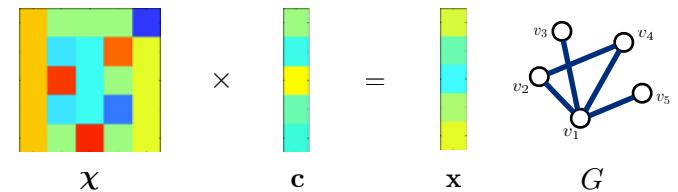


$$\begin{aligned} c_{\text{MAP}}(x) &:= \arg \max_c p(c|x) = \arg \max_c p(x|c)p(c) \\ &= \arg \min_c (-\log p_\epsilon(x - \chi c) - \log p_C(c)) \\ &= \arg \min_c \|x - \chi c\|_2^2 + \alpha c^T \Lambda c \end{aligned}$$

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 \end{aligned}$$

\downarrow

$$\min_{\mathbf{L}, \mathbf{Y}} \|\mathbf{X} - \mathbf{Y}\|_F^2 + \alpha \text{tr}(\mathbf{Y}^T \mathbf{LY}) + \beta \|\mathbf{L}\|_F^2$$

data fidelity

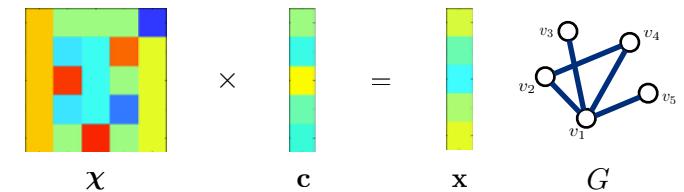
smoothness on \mathbf{Y}

regularization

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$$\min_{\mathbf{L}, \mathbf{Y}} \underbrace{\|\mathbf{X} - \mathbf{Y}\|_F^2}_{\text{data fidelity}} + \alpha \underbrace{\text{tr}(\mathbf{Y}^T \mathbf{LY})}_{\text{smoothness on } \mathbf{Y}} + \beta \underbrace{\|\mathbf{L}\|_F^2}_{\text{regularization}}$$

data fidelity

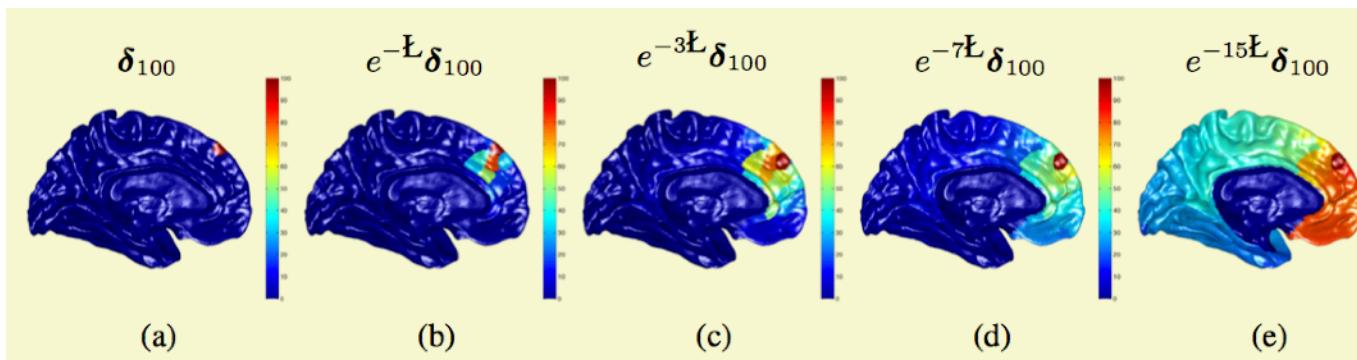
smoothness on \mathbf{Y}

regularization

Learning enforces signal property (global smoothness)!

Model 2: Diffusion process

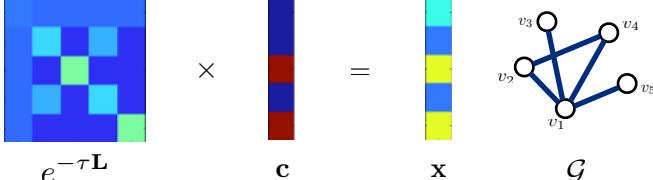
- Signals are the outcome of a diffusion process on the graph (more of local smoothness than global one!)
- Example: Movement of people/ vehicles
- Fully characterized by diffusion operators (graph filters)

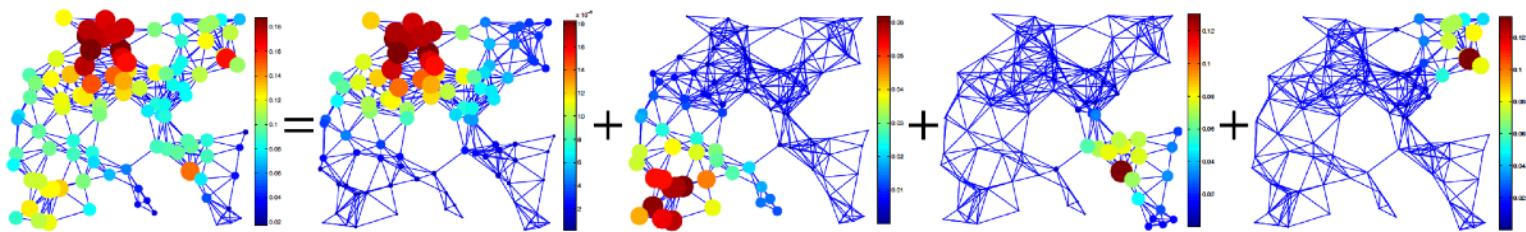


Heat diffusion operators on the brain [7]

Model 2: Diffusion process

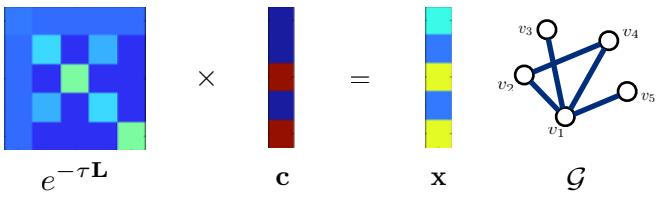
- Thanou et al. (2016)
 - Dictionary of heat diffusion operators
 - Sparsity assumption on c
 - Each signal is a linear combination of heat diffusion processes

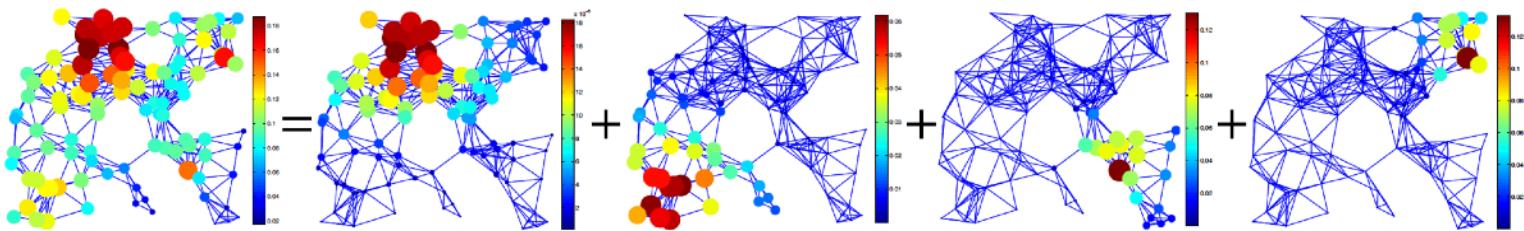
$$e^{-\tau \mathbf{L}} \times \mathbf{c} = \mathbf{x}$$




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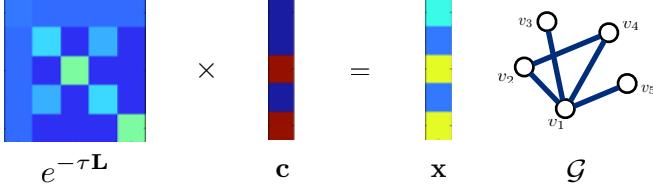
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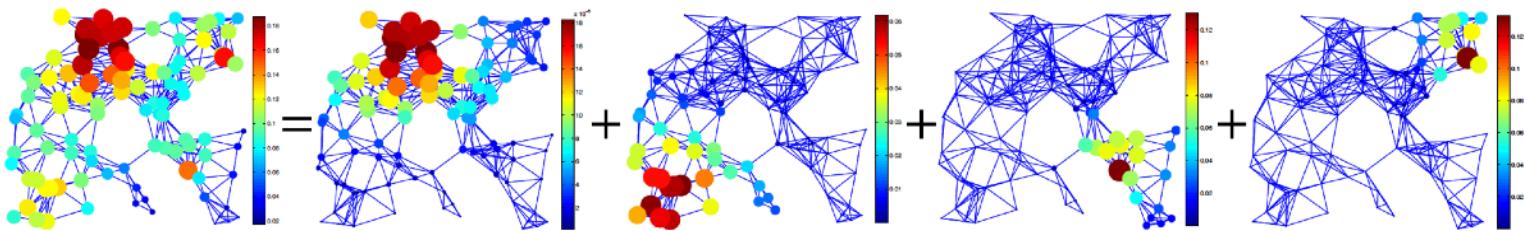


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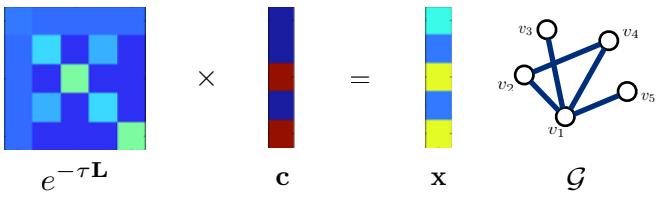
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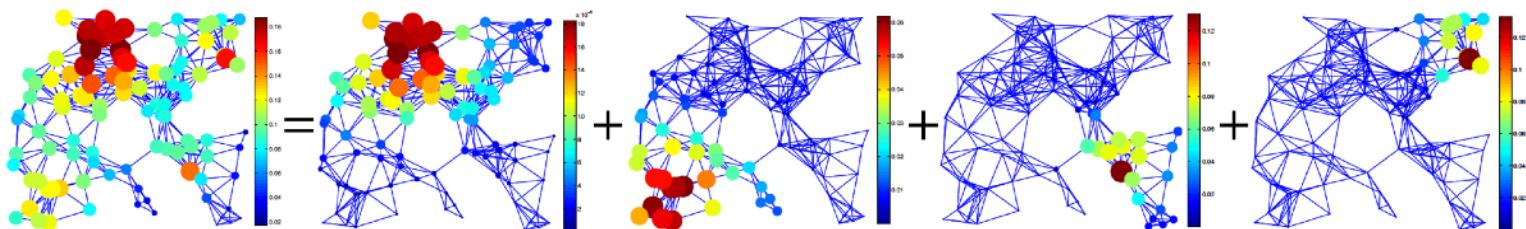


$$\min_{\mathbf{L}, \mathbf{C}, \tau} \|\mathbf{X} - \mathbf{D}(\mathbf{L})\mathbf{C}\|_F^2 + \alpha \sum_{m=1}^M \|\mathbf{c}_m\|_1 + \beta \|\mathbf{L}\|_F^2 \quad \text{s.t.} \quad \mathbf{D} = [e^{-\tau_1 \mathbf{L}}, \dots, e^{-\tau_S \mathbf{L}}]$$

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$$e^{-\tau \mathbf{L}} \times \mathbf{c} = \mathbf{x}$$


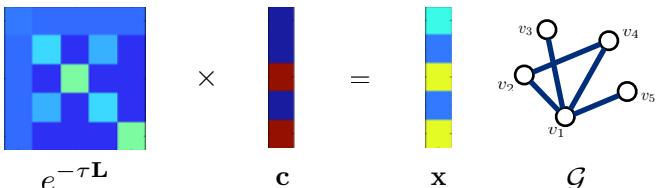


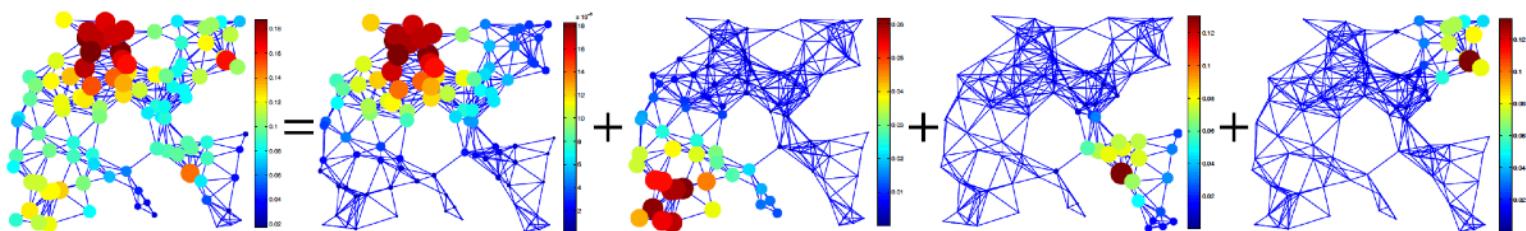
$$\min_{\mathbf{L}, \mathbf{C}, \tau} \|\mathbf{X} - \mathbf{D}(\mathbf{L})\mathbf{C}\|_F^2 + \alpha \sum_{m=1}^M \|\mathbf{c}_m\|_1 + \beta \|\mathbf{L}\|_F^2 \quad \text{s.t.} \quad \mathbf{D} = [e^{-\tau_1 \mathbf{L}}, \dots, e^{-\tau_S \mathbf{L}}]$$

data fidelity sparsity on \mathbf{c} regularization

Model 2: Diffusion process

- Thanou et al. (2016)
 - Dictionary of heat diffusion operators
 - Sparsity assumption on c
 - Each signal is a linear combination of heat diffusion processes

$$e^{-\tau \mathbf{L}} \times \mathbf{c} = \mathbf{x}$$




$$\min_{\mathbf{L}, \mathbf{C}, \tau} \|\mathbf{X} - \mathbf{D}(\mathbf{L})\mathbf{C}\|_F^2 + \alpha \sum_{m=1}^M \|\mathbf{c}_m\|_1 + \beta \|\mathbf{L}\|_F^2 \quad \text{s.t.} \quad \mathbf{D} = [e^{-\tau_1 \mathbf{L}}, \dots, e^{-\tau_S \mathbf{L}}]$$

data fidelity sparsity on \mathbf{c} regularization

Can be extended to general polynomial case (Petric Maretic et al. 2017)

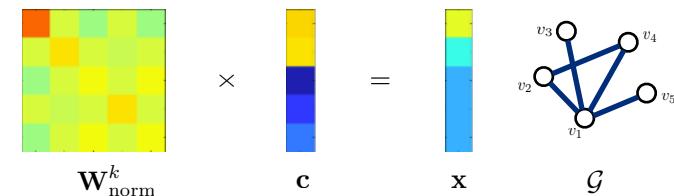
Model 2: Diffusion process

- Pasdeloup et al. (2016), Segarra et al. (2016)

- Dictionary: powers of the normalized weight matrix

$$\mathbf{D}(\mathcal{G}) = \mathbf{T}^{\mathbf{k}(m)} = \mathbf{W}_{\text{norm}}^{\mathbf{k}(m)}$$

- i.i.d. assumption on the coefficients c



- Two stage approach for estimating the topology:

- Estimate the eigenvectors from the sample covariance

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

- Optimize the eigenvalues given constraints on the topology (sparsity, non-negativity)

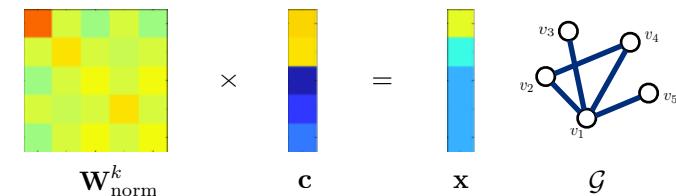
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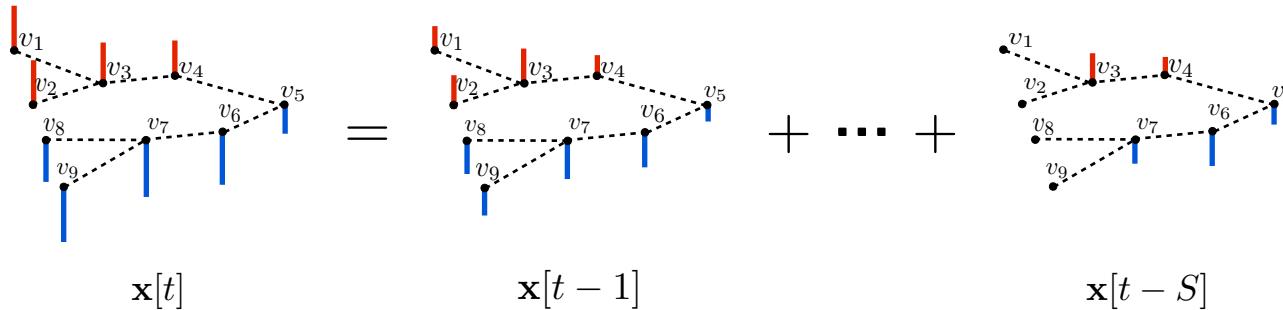
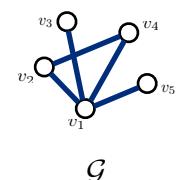
More a “graph-centric” framework: Cost on graph components instead of signals

Model 3: Time varying signals

- Mei et al. (2016)

- $D_s(G) = P_s(W)$: polynomial of W of degree s
- Define $c_s = x[t - s]$

$$\Sigma_{s=1}^S \left(\begin{array}{c|ccccc} & & & & \\ & & & & \\ & & & & \\ \textbf{P}_s(\mathbf{W}) & \textcolor{red}{\blacksquare} & \textcolor{blue}{\blacksquare} & \textcolor{cyan}{\blacksquare} & \textcolor{yellow}{\blacksquare} \\ & & & & \\ & & & & \end{array} \right) \times \begin{array}{c} \textcolor{red}{\square} \\ \textcolor{blue}{\square} \\ \textcolor{cyan}{\square} \\ \textcolor{yellow}{\square} \end{array} = \begin{array}{c} \textcolor{green}{\square} \\ \textcolor{cyan}{\square} \\ \textcolor{yellow}{\square} \\ \textcolor{green}{\square} \end{array} \mathbf{x}$$



$$\min_{\mathbf{W}, \mathbf{a}} \frac{1}{2} \sum_{k=S+1}^K \left(\left\| \mathbf{x}[k] - \sum_{s=1}^S \mathbf{P}_s(\mathbf{W}) \mathbf{x}[k-s] \right\|_2^2 + \lambda_1 \|\text{vec}(\mathbf{W})\|_1 + \lambda_2 \|\mathbf{a}\|_1 \right)$$

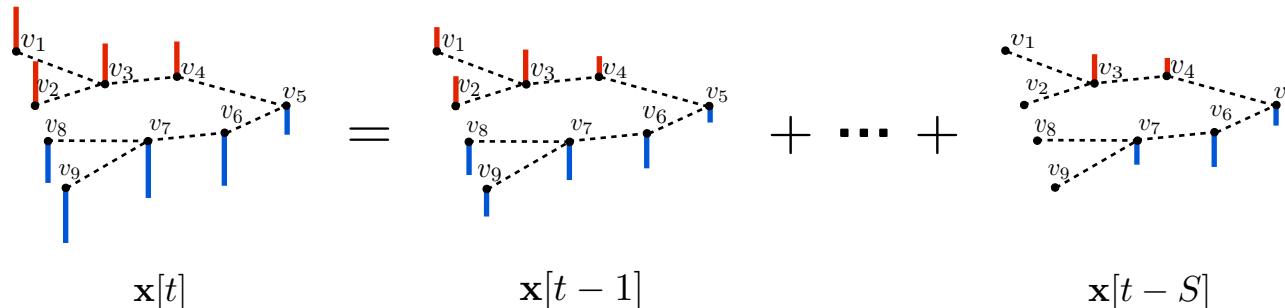
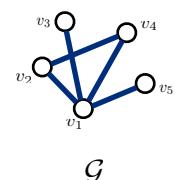
data fidelity sparsity on \mathbf{W} sparsity on \mathbf{a}

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$$\min_{\mathbf{W}, \mathbf{a}} \frac{1}{2} \sum_{k=S+1}^K \left(\|\mathbf{x}[k] - \sum_{s=1}^S \textbf{P}_s(\mathbf{W}) \mathbf{x}[k-s]\|_2^2 + \lambda_1 \|\text{vec}(\mathbf{W})\|_1 + \lambda_2 \|\mathbf{a}\|_1 \right)$$

data fidelity

sparsity on \mathbf{W}

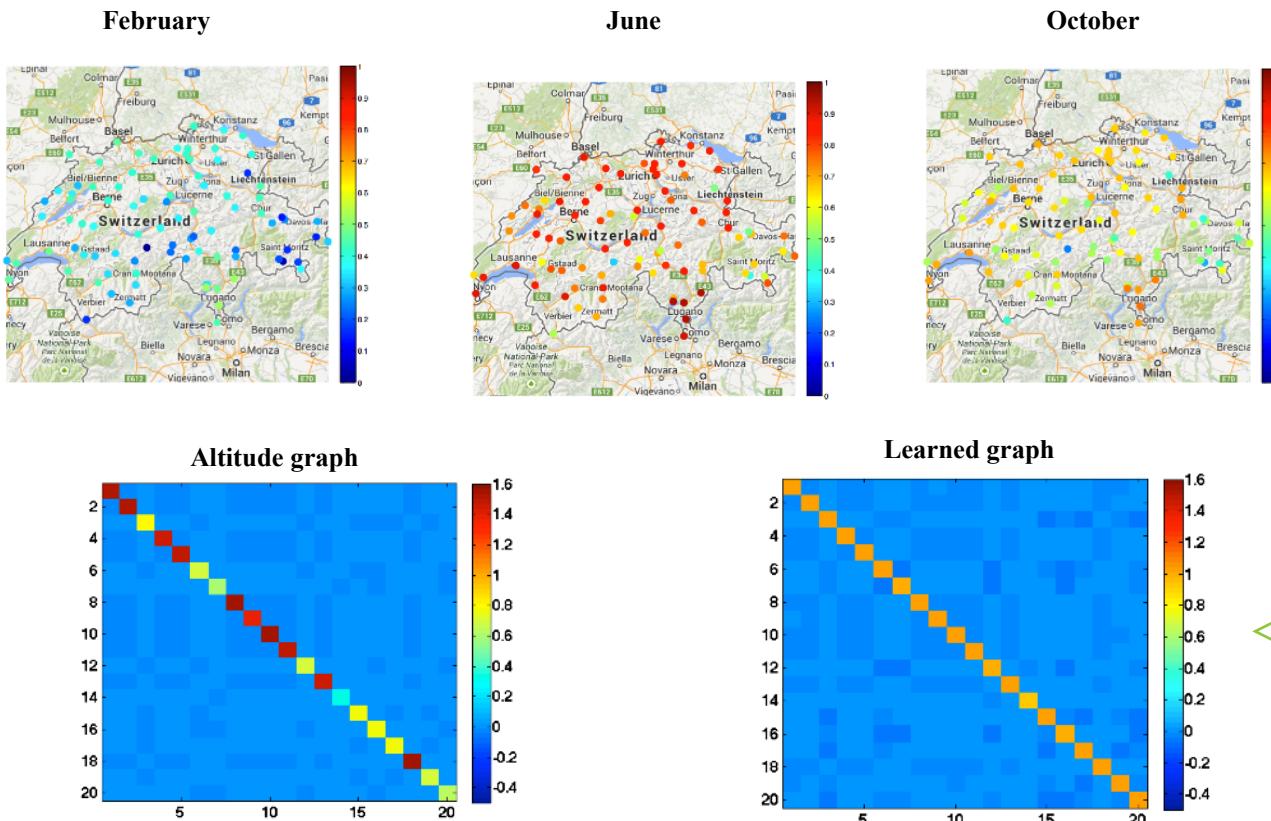
sparsity on \mathbf{a}

Good for inferring causal relations between signals

Kernel version (nonlinear): Shen et al. (2016)

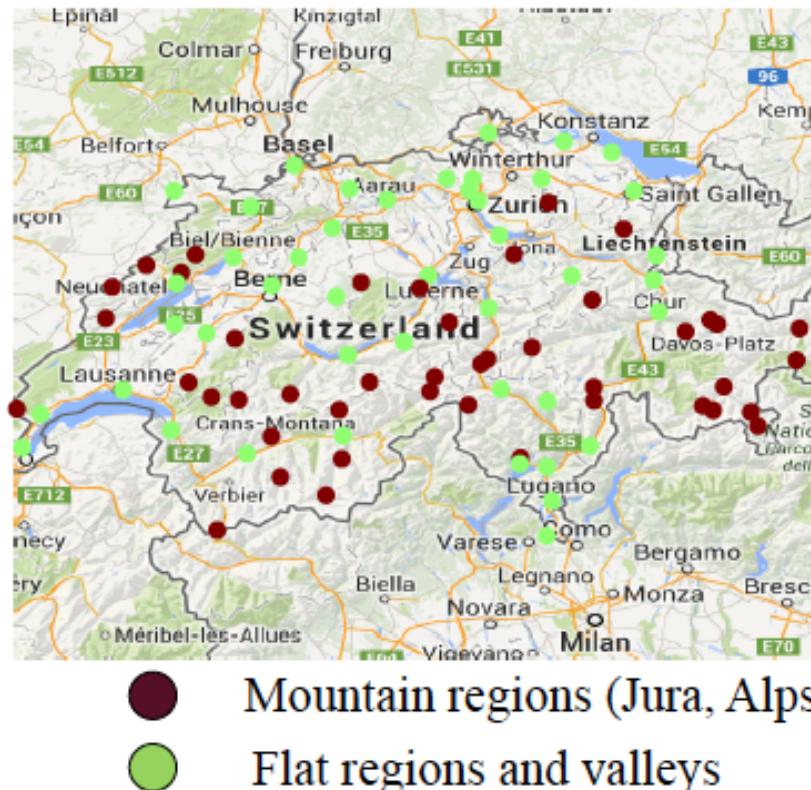
Application 1: Understanding meteorological data

- Signals: 12 monthly temperature records at 89 measuring stations [9]



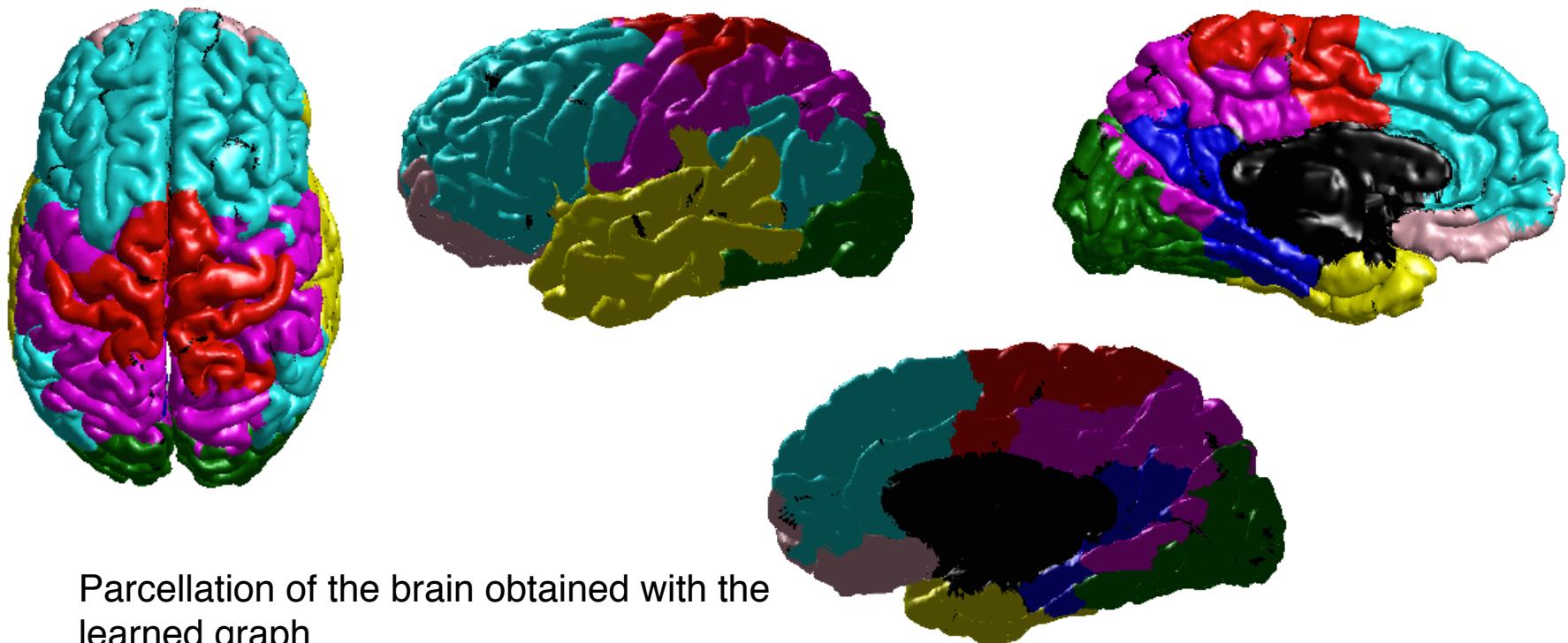
Application 1: Understanding meteorological data

- The learned graph can be used for partitioning nodes into several clusters:



Application 2: Infer brain connections

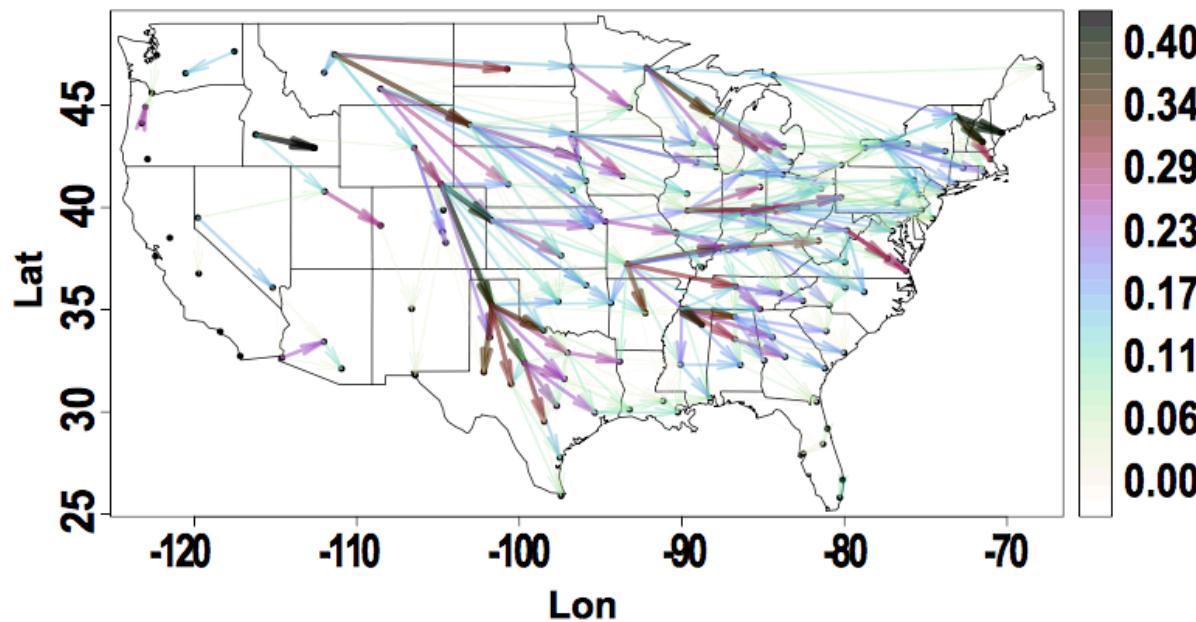
- Signals: time series recorded in MRI scan while the subjects are at rest



Parcellation of the brain obtained with the learned graph

Application 3: Learning wind directions

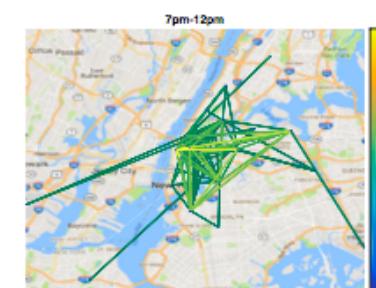
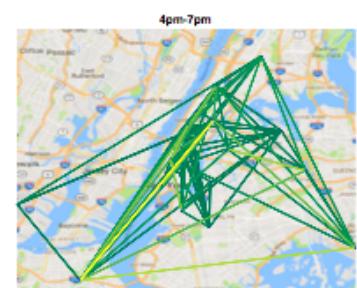
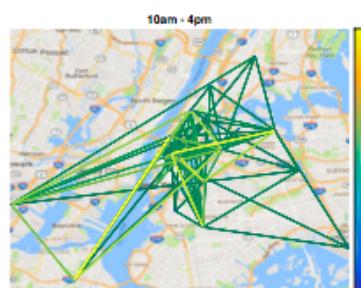
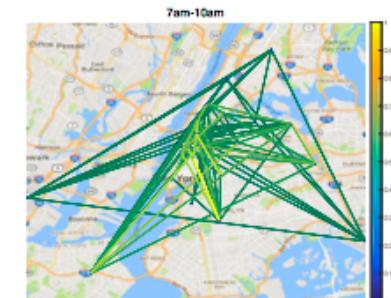
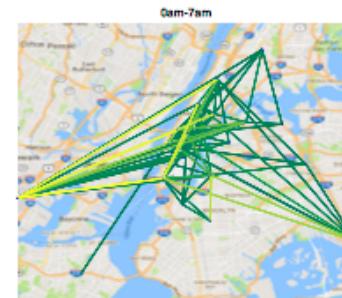
- Signals: daily temperature taken over 365 days at 150 cities in USA [20]



- The graph learned the predominant west-to-east and north-northwest-to-south-southeast directions

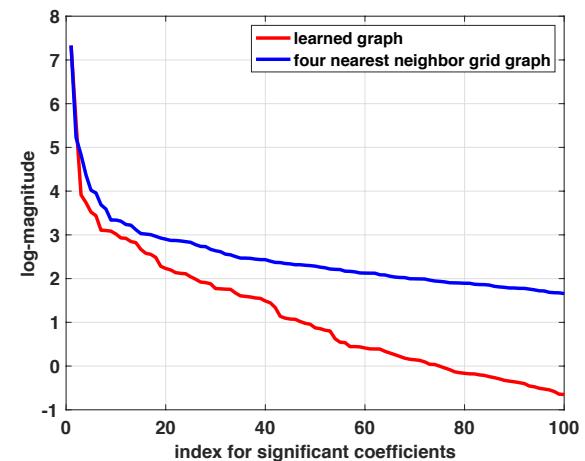
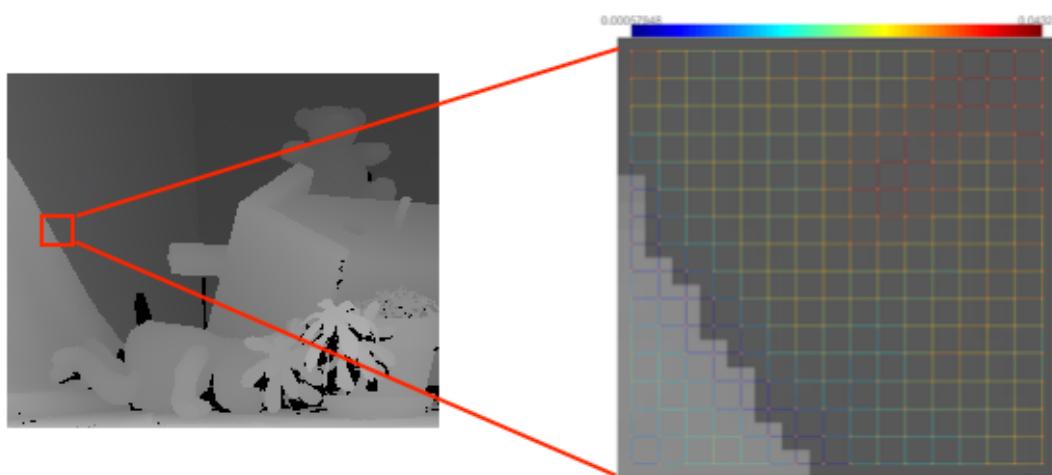
Application 4: Mining traffic behavior

- Learn the traffic patterns in NCY using a heat diffusion model [35]
 - nodes: centroids of taxi zones
 - signals: the hourly number of Uber pickups in each zone



Application 5: Image coding

- Graph learning can be used for efficient coding of image signals
- Additional constraints can be used to reduce the transmission cost of the graph



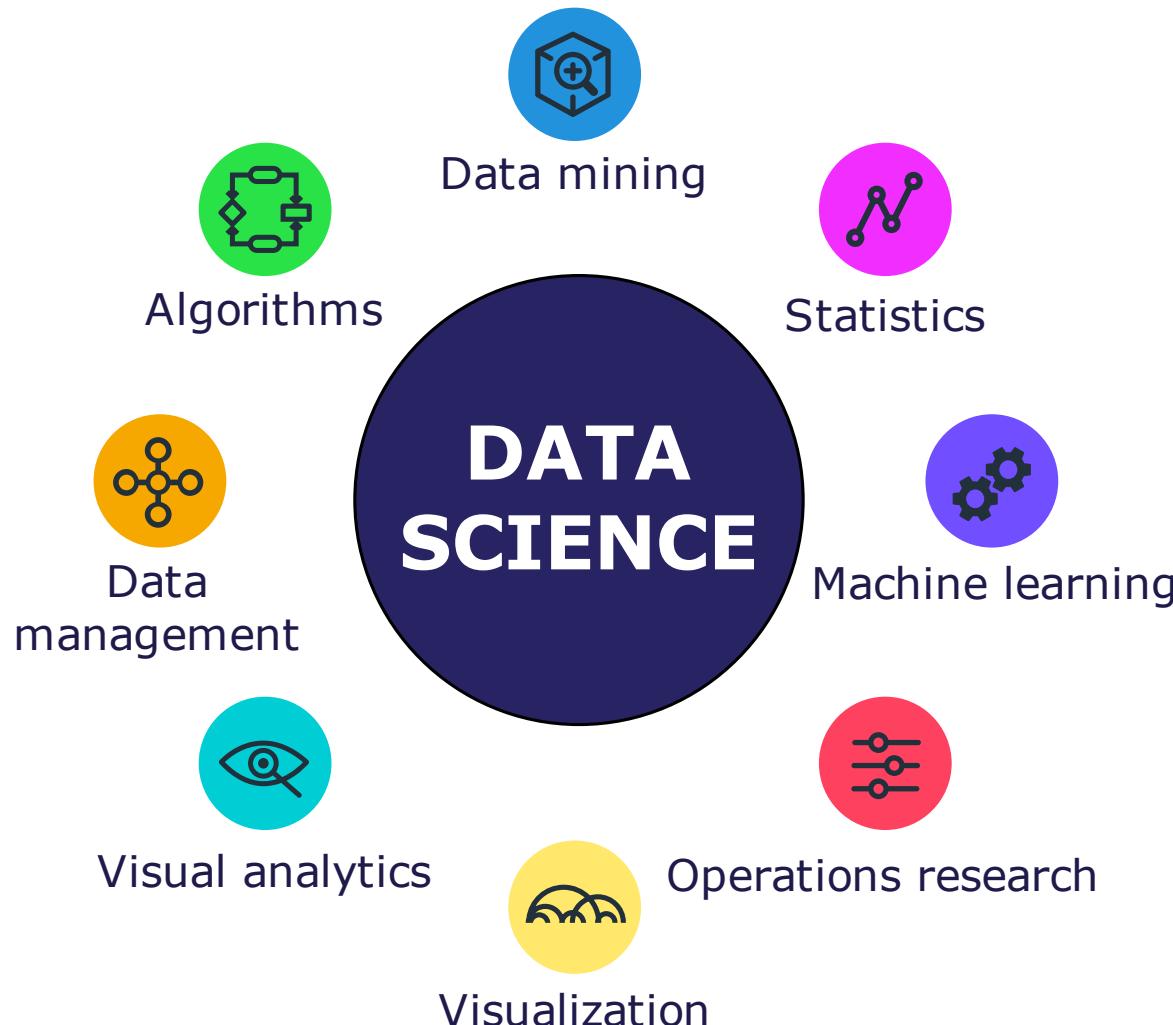
Comparison of GSP methods

| Methods | Signal model | Assumption | Learning output | Edge direction | Inference |
|------------------|--------------------------|------------------------------|---------------------------|----------------|----------------|
| Dong (2015) | Global smoothness | Gaussian | Laplacian | Undirected | Signal-centric |
| Thanou (2016) | Heat diffusion | Sparsity | Laplacian | Undirected | Signal-centric |
| Pasdeloup (2015) | Diffusion by Adj. matrix | Stationary | Normalised Adj./Laplacian | Undirected | Graph-centric |
| Mei (2015) | Time-varying | Dependent on previous states | Adj. matrix | Directed | Signal-centric |

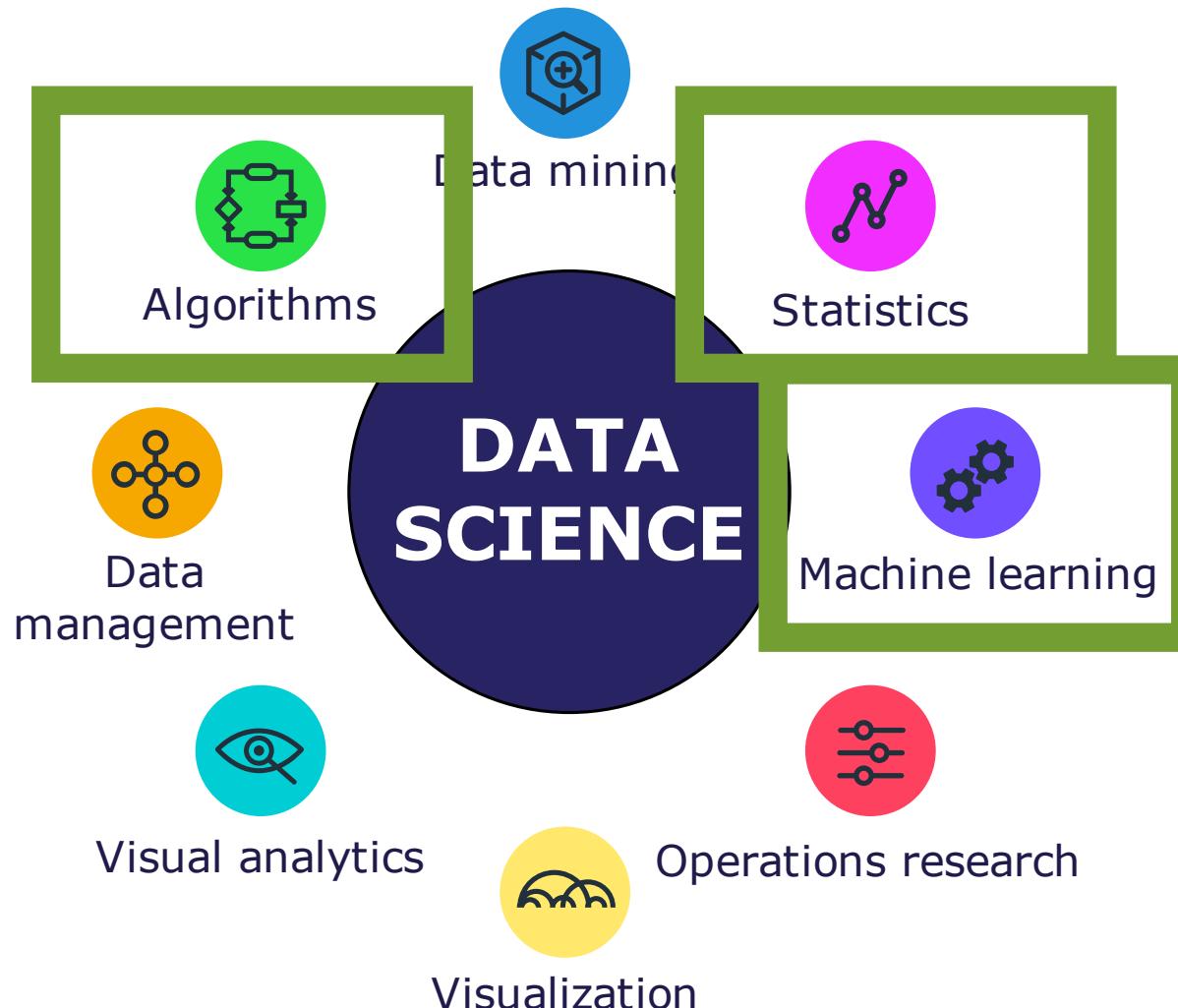
Take-home messages

- Data is often structured
- **Graphs:** a flexible tool for modeling many real-world data
- If the structure if not known, **learn** it from the data
- The choice of the learning algorithm depends on many parameters (signal model, application)

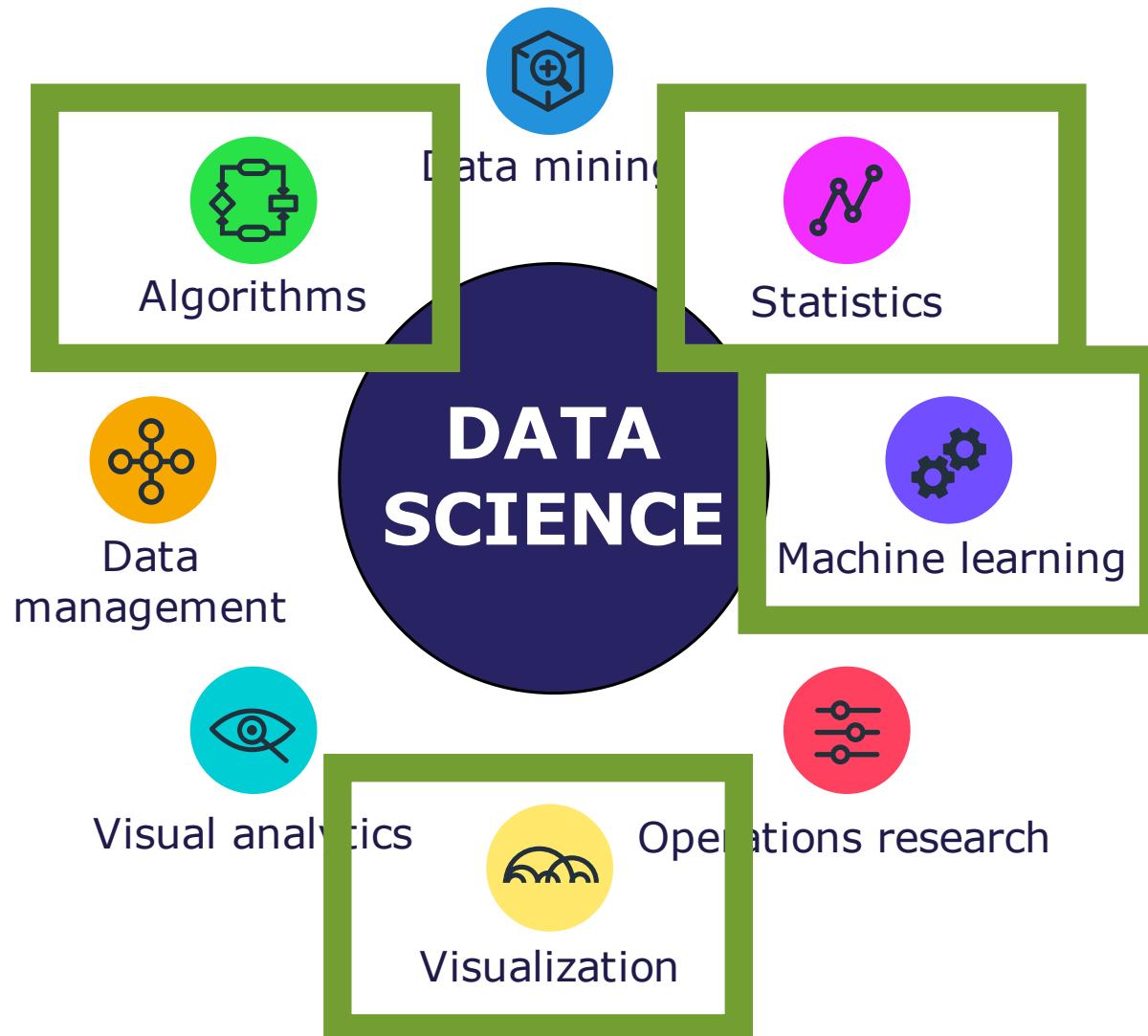
Network inference: Powerful tool for Data Science



Network inference: Powerful tool for Data Science



Network inference: Powerful tool for Data Science



Overview paper

1

Learning Graphs from Data: A Signal Representation Perspective

Xiaowen Dong*, Dorina Thanou*, Michael Rabbat, and Pascal Frossard

The construction of a meaningful graph topology plays a crucial role in the effective representation, processing, analysis and visualization of structured data. When a natural choice of the graph is not readily available from the datasets, it is thus desirable to infer or learn a graph topology from the data. In this tutorial overview, we survey solutions to the problem of graph learning, including classical viewpoints from statistics and physics, and more recent approaches that adopt a graph signal processing (GSP) perspective. We further emphasize the conceptual similarities and differences between classical and GSP graph inference methods and highlight the potential advantage of the latter in a number of theoretical and practical scenarios. We conclude with several open issues and challenges that are keys to the design of future signal processing and machine learning algorithms for learning graphs from data.

I. INTRODUCTION

Modern data analysis and data processing tasks typically involve large sets of structured data, where the structure carries critical information about the nature of the data. One can find numerous examples of such datasets in a wide diversity of application domains, including transportation networks, social networks, computer networks, and brain networks. Typically, graphs are used as mathematical tools to describe the structure of such data. They provide a flexible way for representing relationships between data entities. Numerous signal processing and machine learning algorithms have been introduced in the past decade for analyzing structured data on *a priori* known graphs [1], [2]. However, there are often settings where the graph is not readily available, and the structure of the data has to be estimated in order to permit effective representation, processing, analysis or visualization of graph data. In this case, a crucial task is to infer a graph topology that describes the characteristics of the data observations, hence capturing the underlying relationship between these entities.

The problem of graph learning is the following: given M observations of N variables or data entities, represented in a data matrix $\mathbf{X} \in \mathbb{R}^{N \times M}$, and given some prior knowledge (e.g., distribution, data model,

*Authors contributed equally.

QUESTIONS?



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