

Learning Graphs From Data

A Signal Processing Perspective

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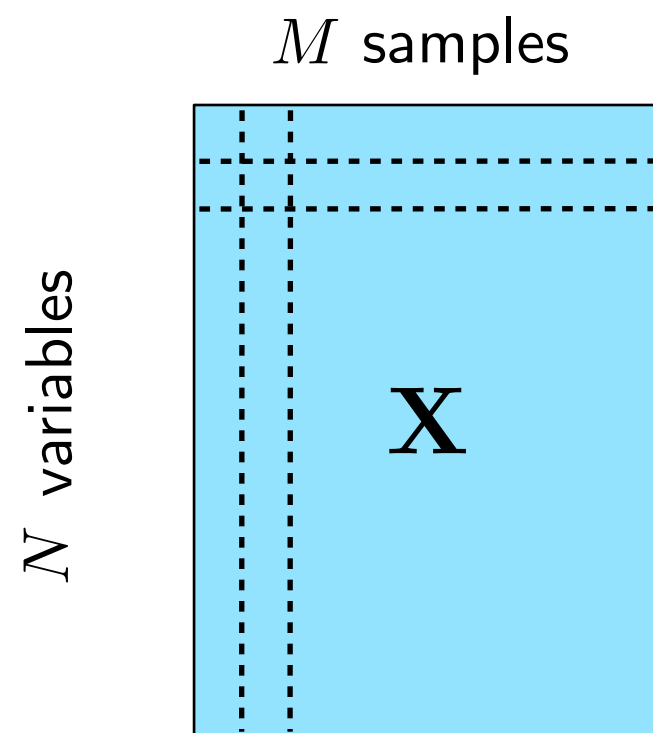


Introduction

- What is the problem of graph learning?

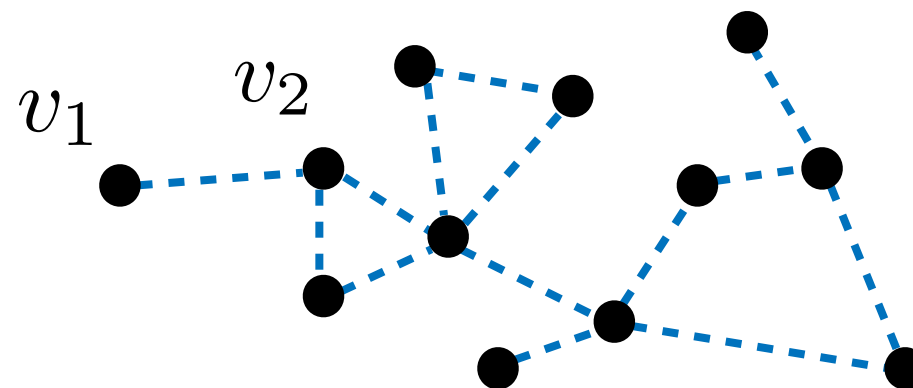
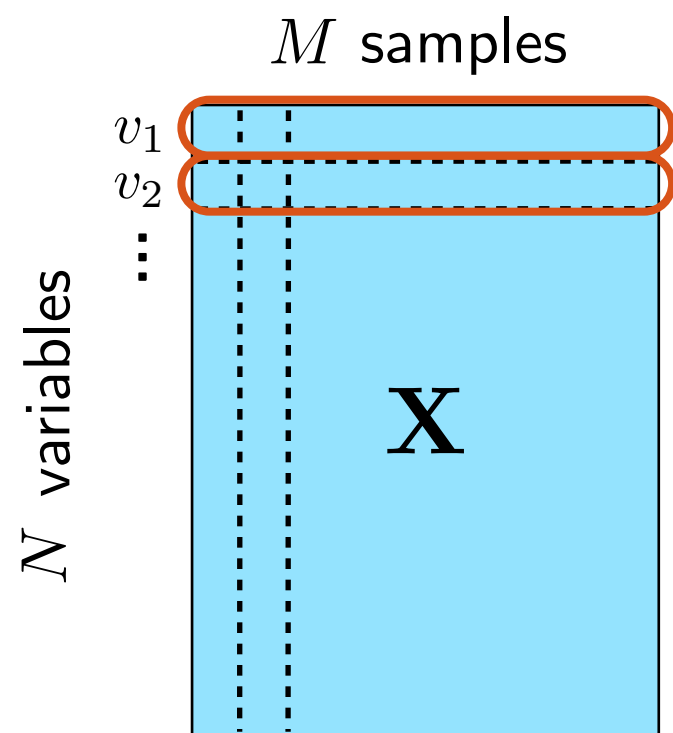
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 - given observations on a number of variables and some prior knowledge (distribution, model, etc)



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 - given observations on a number of variables and some prior knowledge (distribution, model, etc)
 - build/learn a measure of pairwise relation between variables (correlation/covariance, graph topology/operator or equivalent)



Introduction

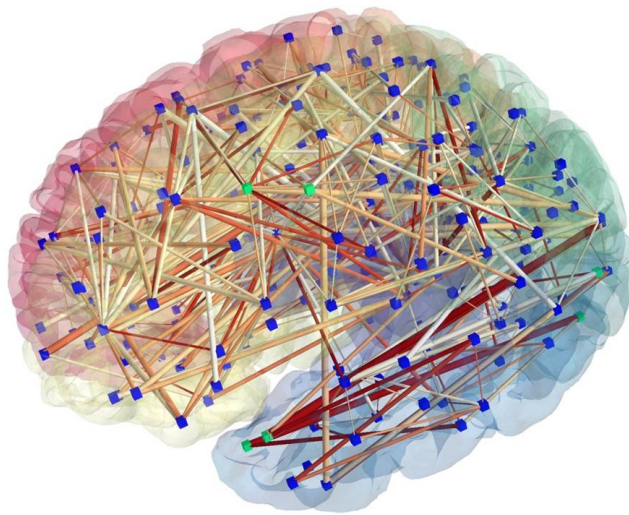
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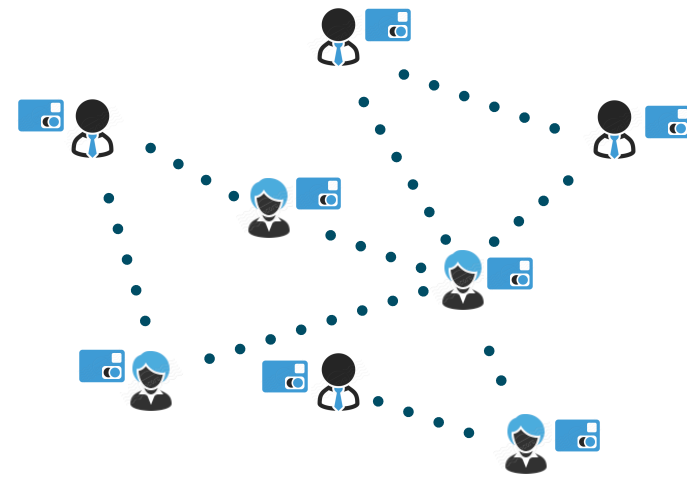
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Input: fMRI recordings in brain regions

Objective: functional connectivity
between brain regions

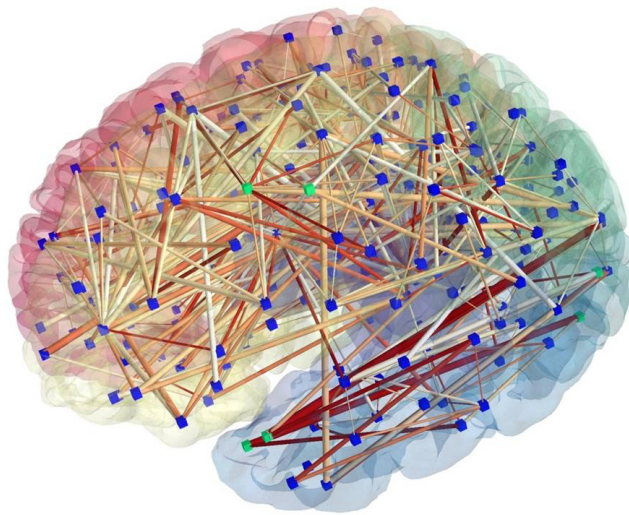


Input: history of individual activities

Objective: behavioural similarity/
influence between people

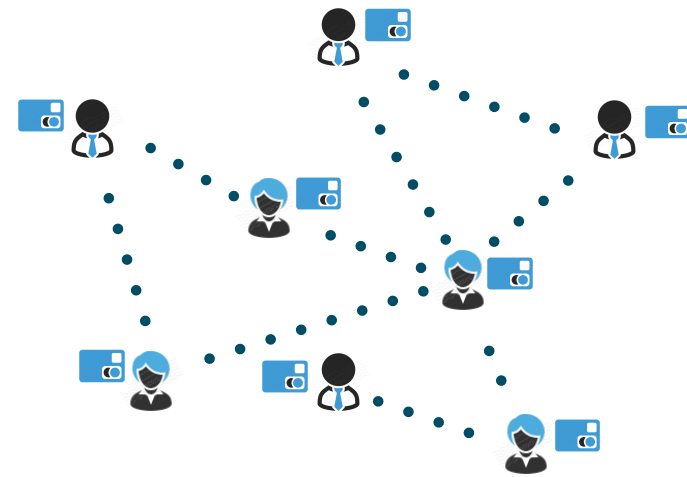
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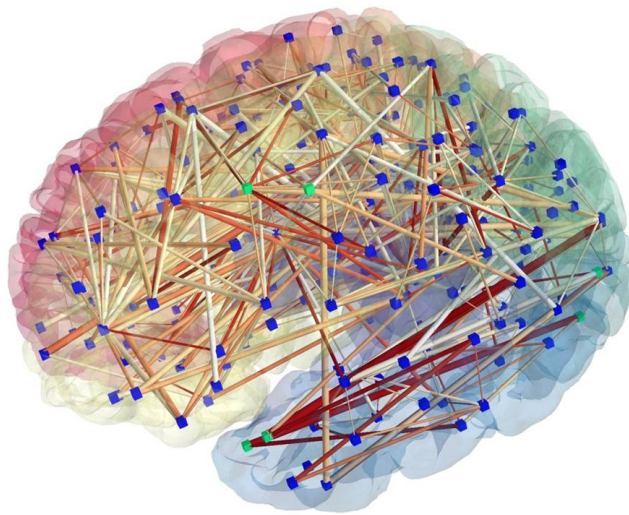


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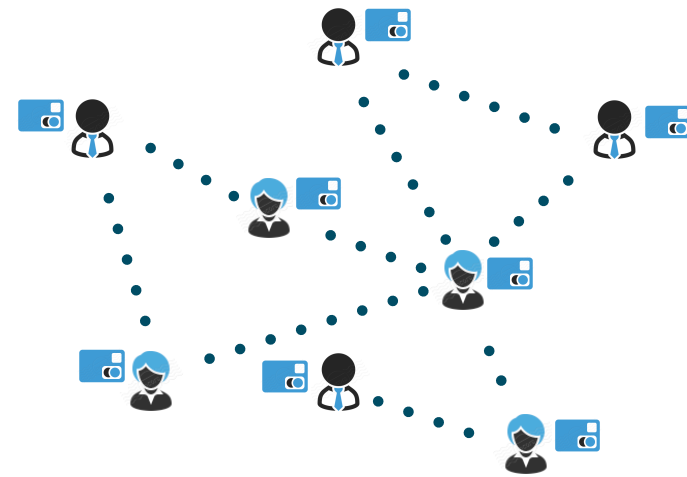
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how do we build/learn the graph?

Outline

- A (very partial) literature overview
- A signal processing perspective
 - A brief introduction to graph signal processing (GSP)
 - GSP approaches for graph learning
- Concluding remarks

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 - sample correlation
 - similarity function (e.g., Gaussian RBF)

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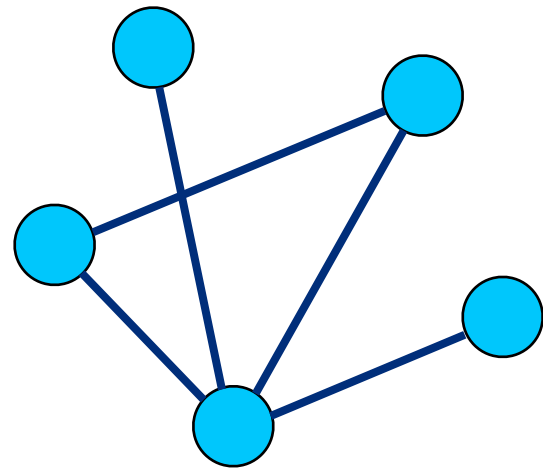
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A (very partial) literature overview

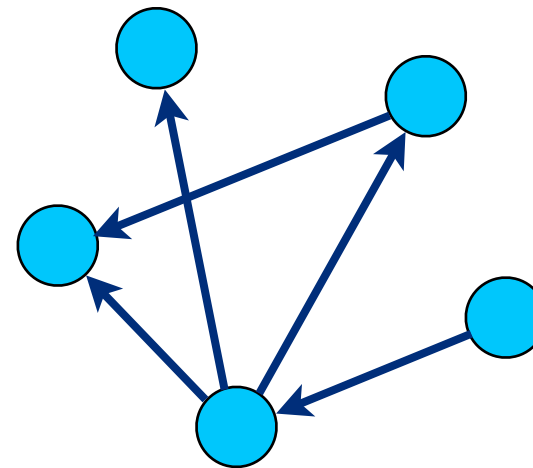
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 - **statistical models**: \mathbf{F} draws realisations from a distribution determined by \mathbf{G} (e.g., probabilistic graphical models)
 - **physically motivated models**: \mathbf{F} is based on a physical generative process on \mathbf{G} (e.g., diffusion processes on graphs)

A (very partial) literature overview

- Learning graphical models



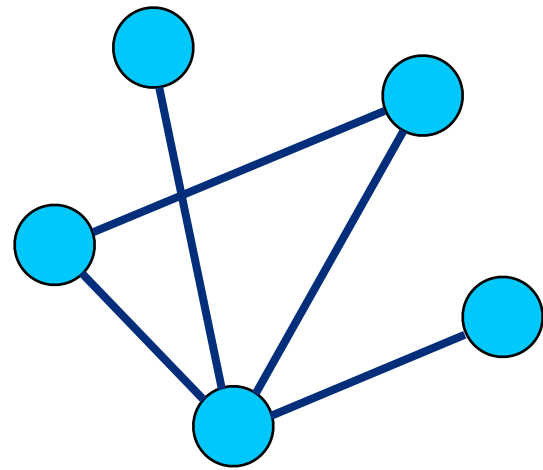
undirected graphical models:
Markov random fields (MRFs)



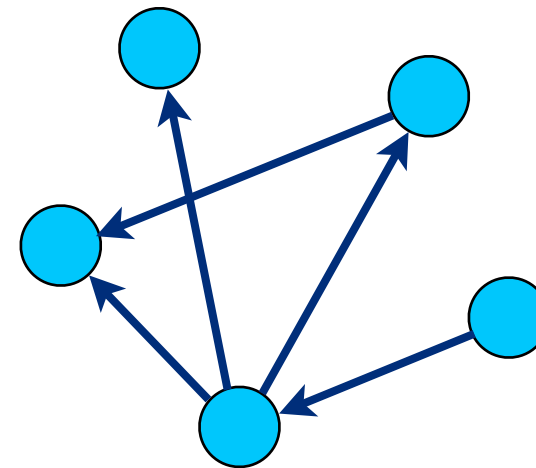
directed graphical models:
Bayesian networks (BNs)

A (very partial) literature overview

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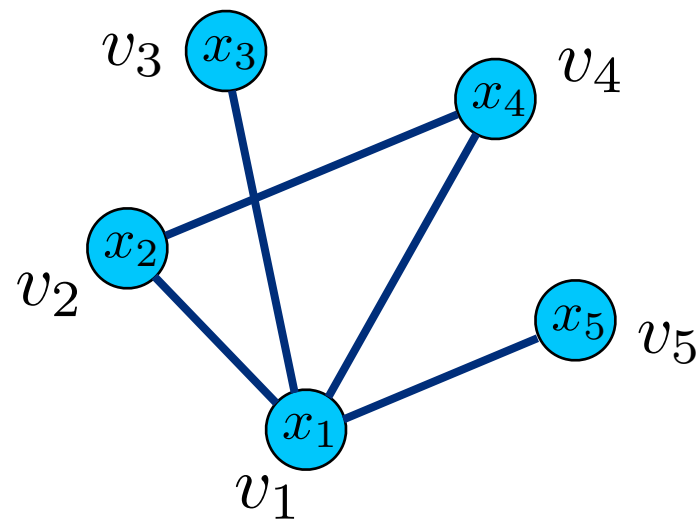
- Learning pairwise MRF

A (very partial) literature overview

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conditional independence:

$$(v_i, v_j) \notin \mathcal{E} \Leftrightarrow x_i \perp x_j \mid \mathbf{x} \setminus \{x_i, x_j\}$$



A (very partial) literature overview

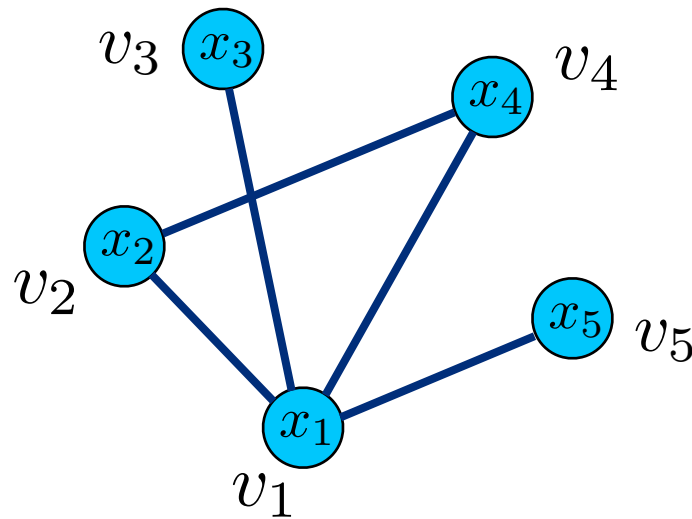
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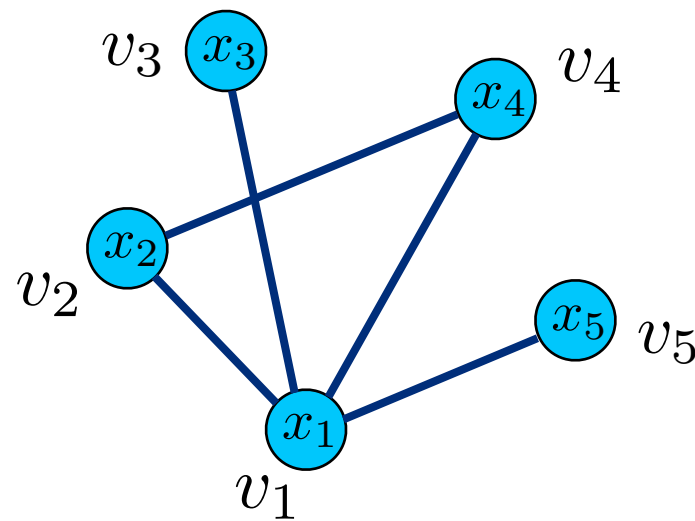
probability parameterised by Θ :

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



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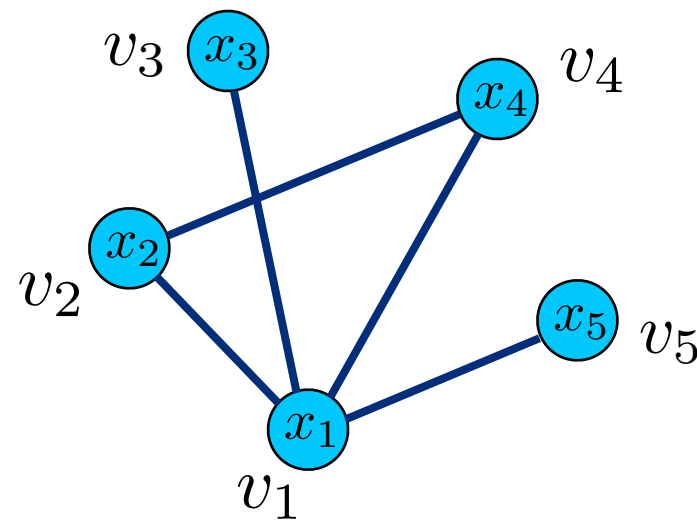
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$$P(\mathbf{x}|\Theta) = \frac{|\Theta|^{1/2}}{(2\pi)^{N/2}} \exp\left(-\frac{1}{2} \mathbf{x}^T \Theta \mathbf{x}\right)$$

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learning a sparse Θ :

- interactions are mostly local
- feasible in high-dimensional space

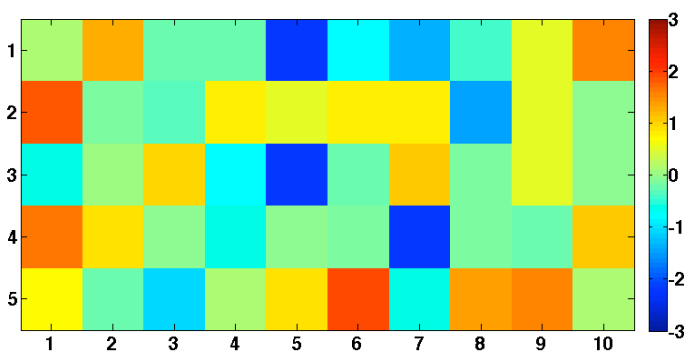
A (very partial) literature overview

*covariance
selection*

Dempster



1972



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

data matrix

A (very partial) literature overview

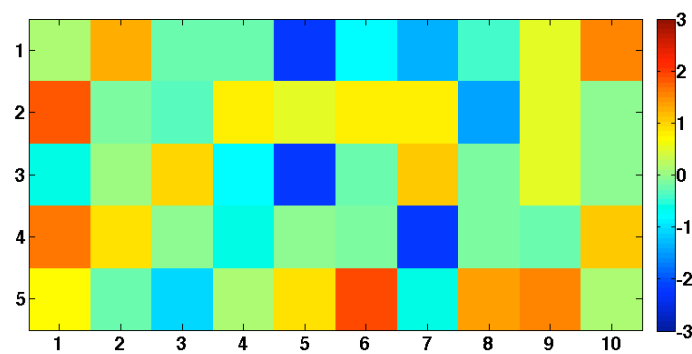
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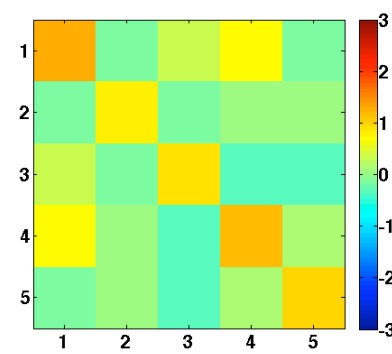
1972

choosing covariance that agrees with \mathbf{S} in set J (precision is zero in complementary set I)



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\mathbf{S}

sample covariance

A (very partial) literature overview

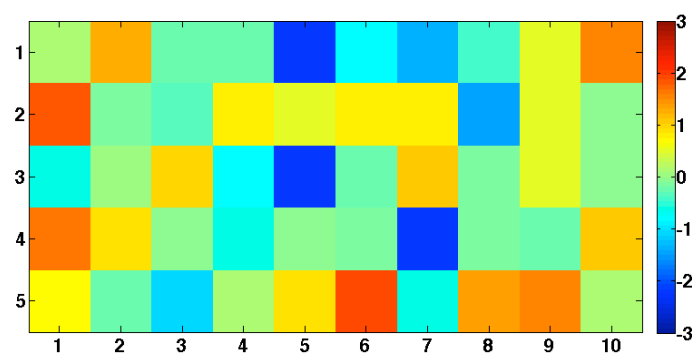
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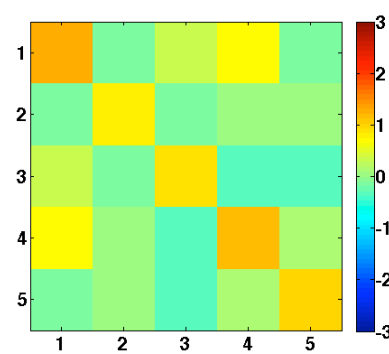
1972

sequentially pruning elements in set I in sample precision



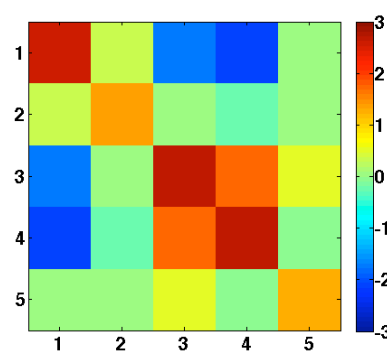
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\mathbf{S}^{-1}

sample precision

A (very partial) literature overview

covariance
selection

ℓ_1 -regularised
neighbourhood
regression

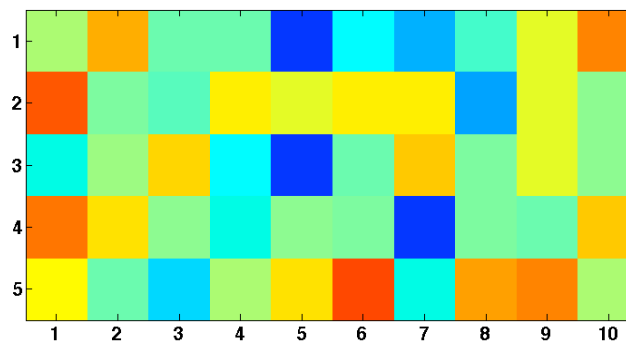
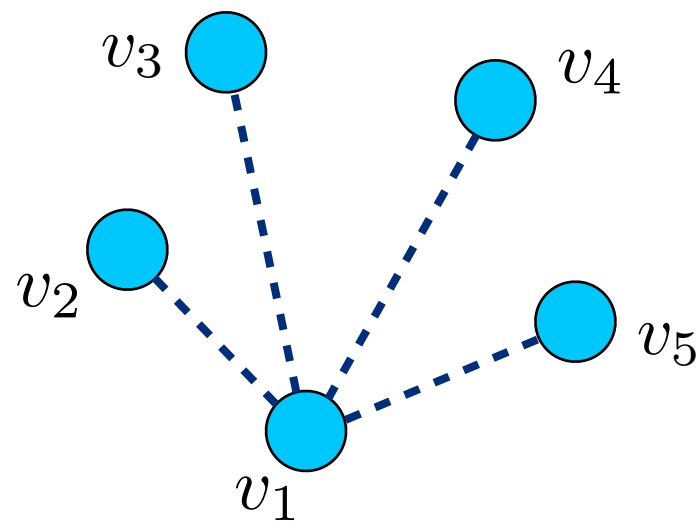
Dempster

Meinshausen
& Bühlmann

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neighbourhood selection: learning neighbourhood of each node



A (very partial) literature overview

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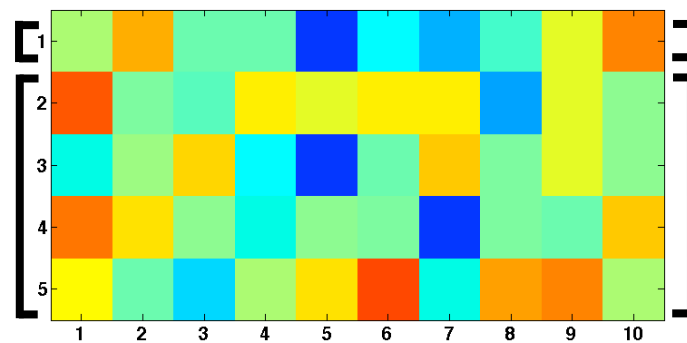
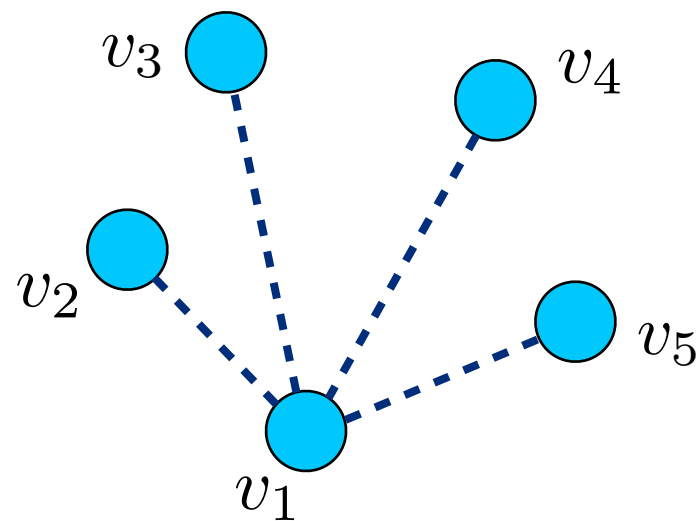
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\mathbf{X}_1^T

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

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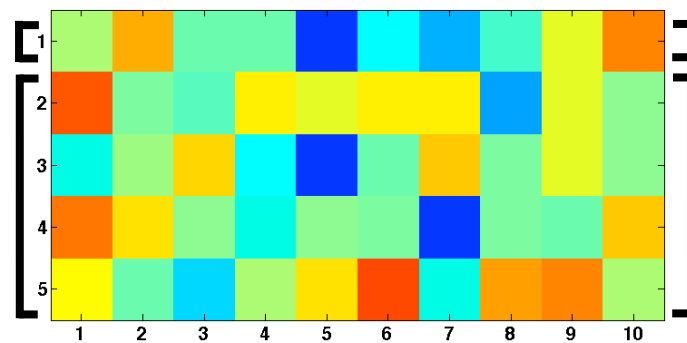
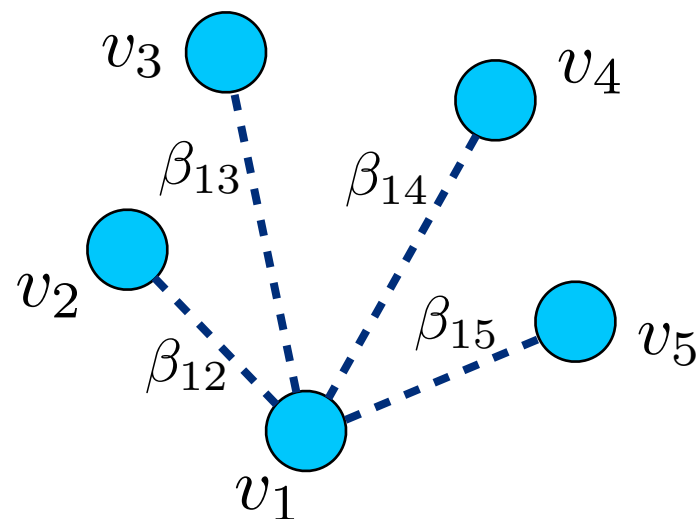
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Lasso regression: $\min_{\boldsymbol{\beta}_1} ||\mathbf{X}_1 - \mathbf{X}_{\setminus 1}\boldsymbol{\beta}_1||^2 + \lambda||\boldsymbol{\beta}_1||_1$

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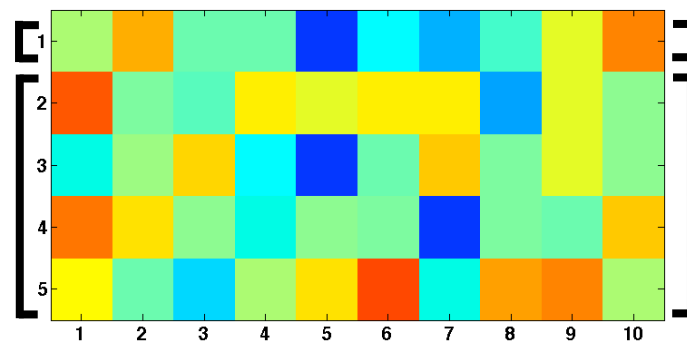
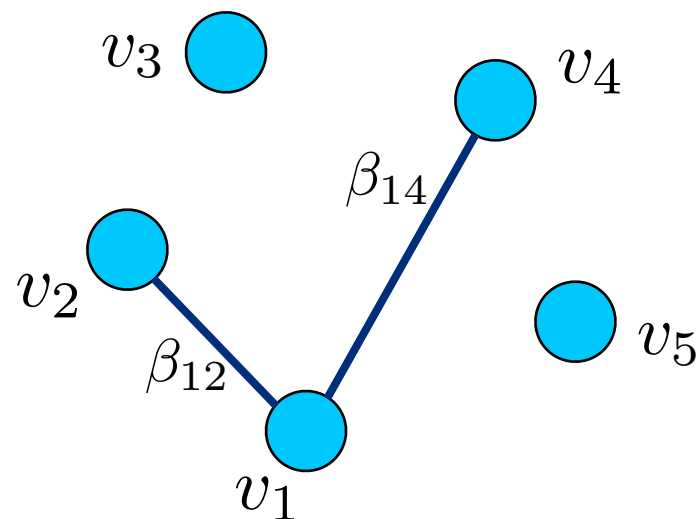
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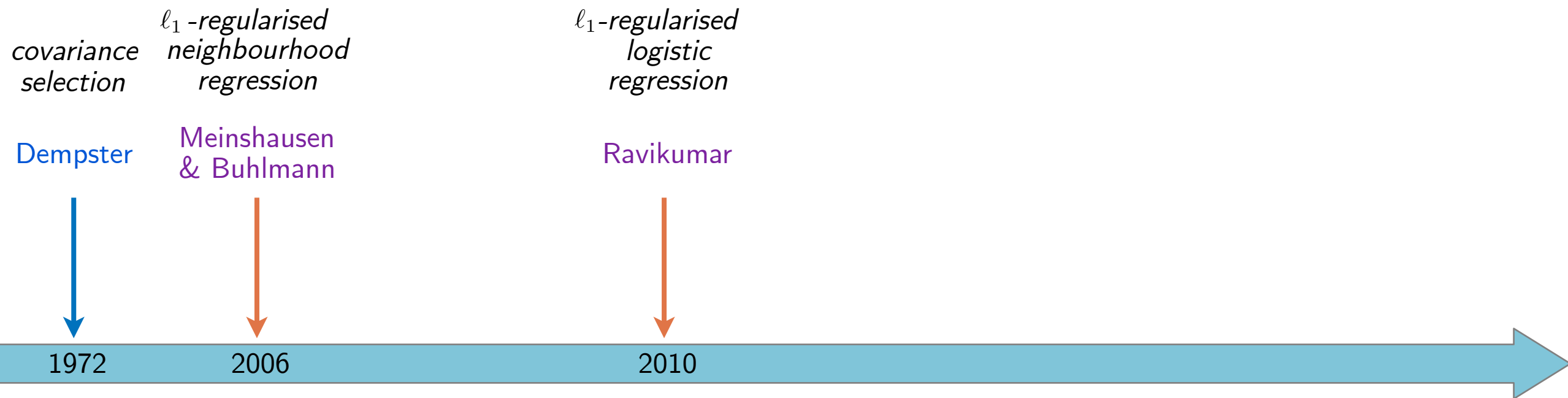


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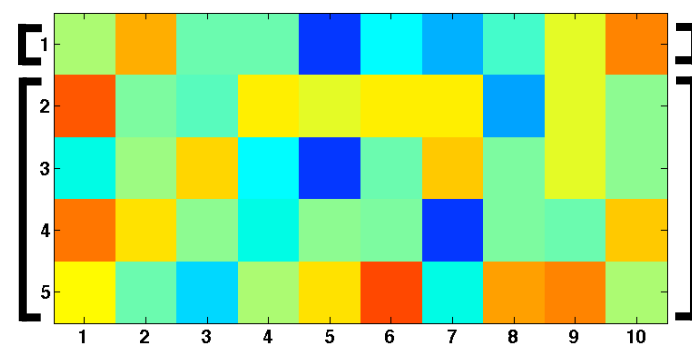
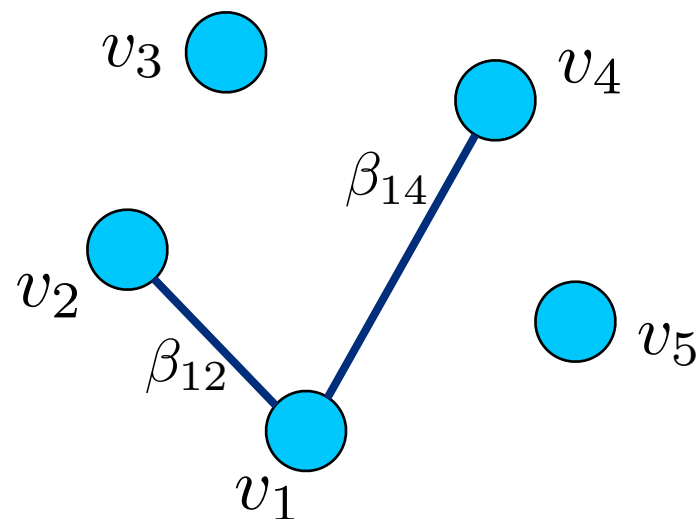
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A (very partial) literature overview



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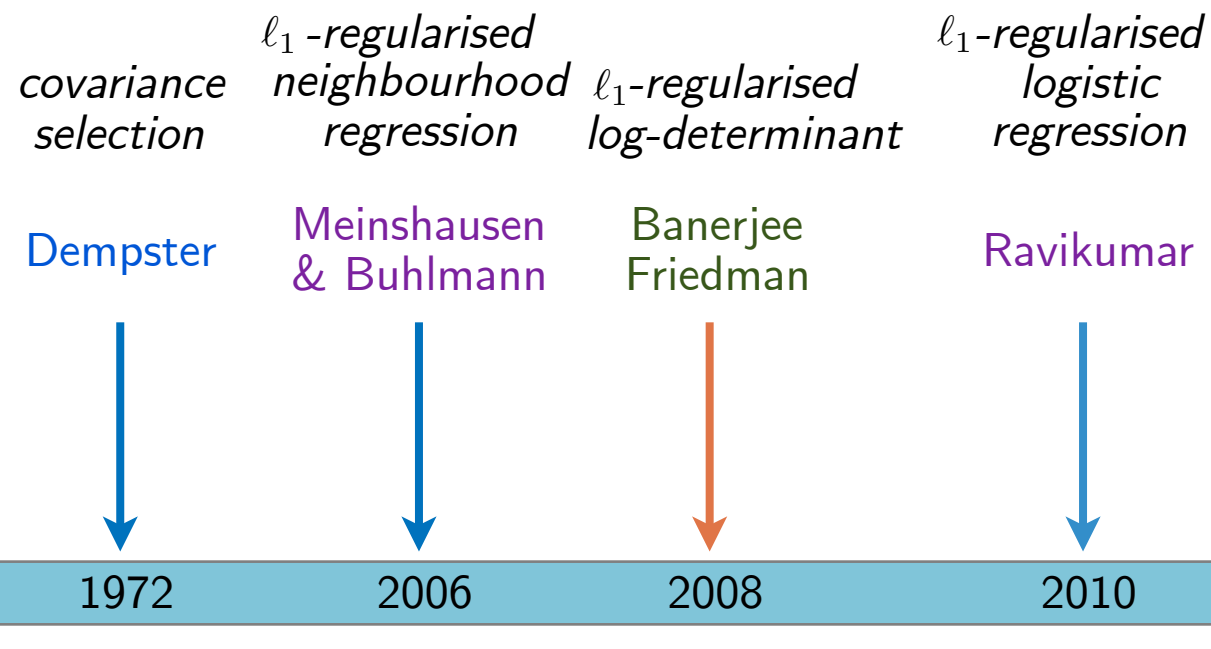
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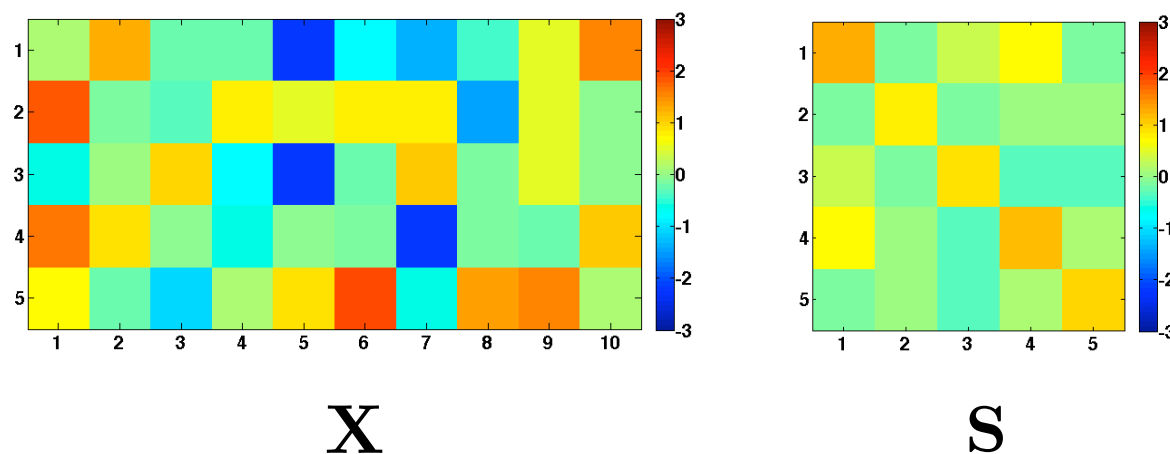
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logistic regression for discrete variables

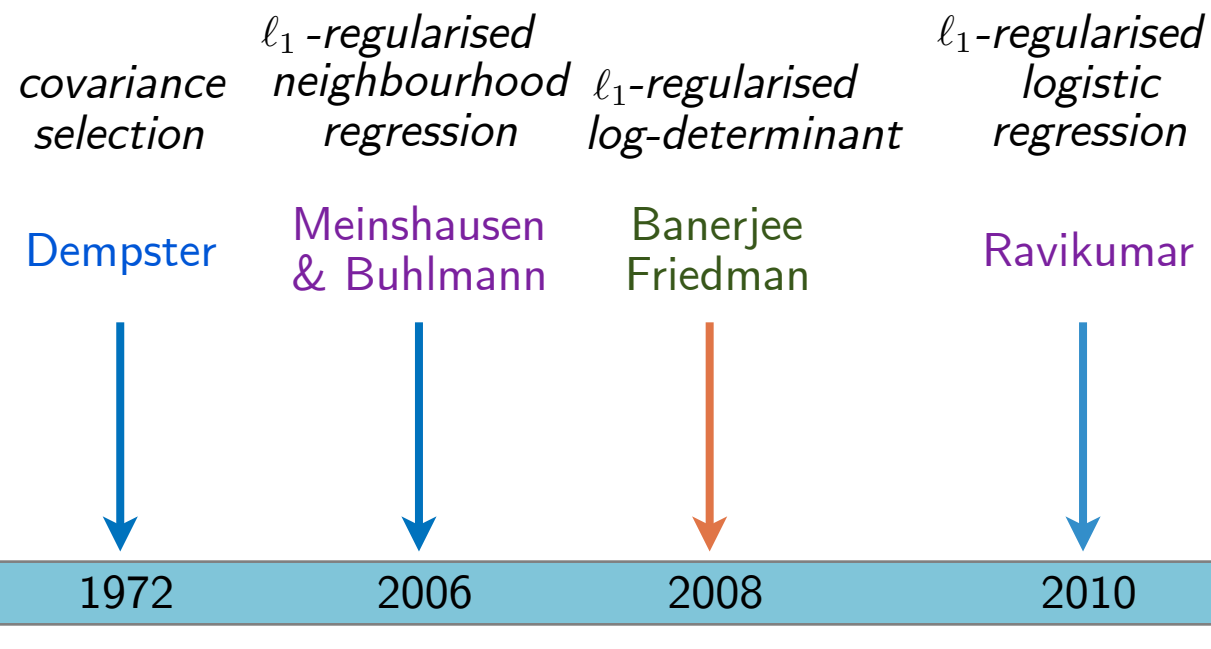
A (very partial) literature overview



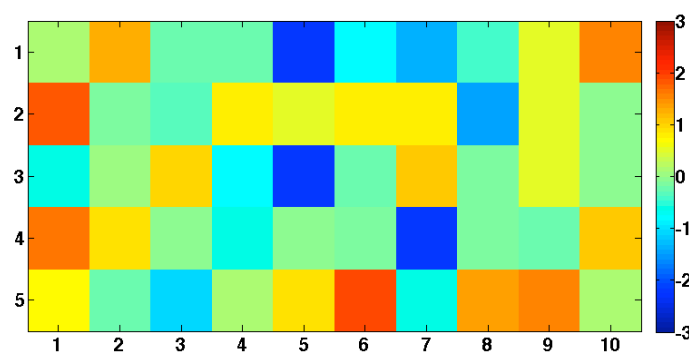
graphical Lasso: estimation of sparse precision matrix



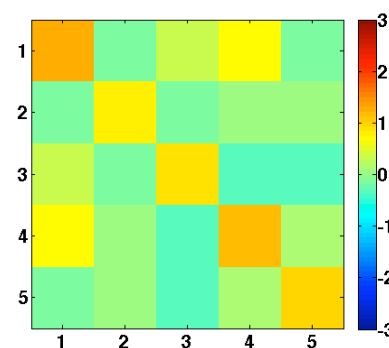
A (very partial) literature overview



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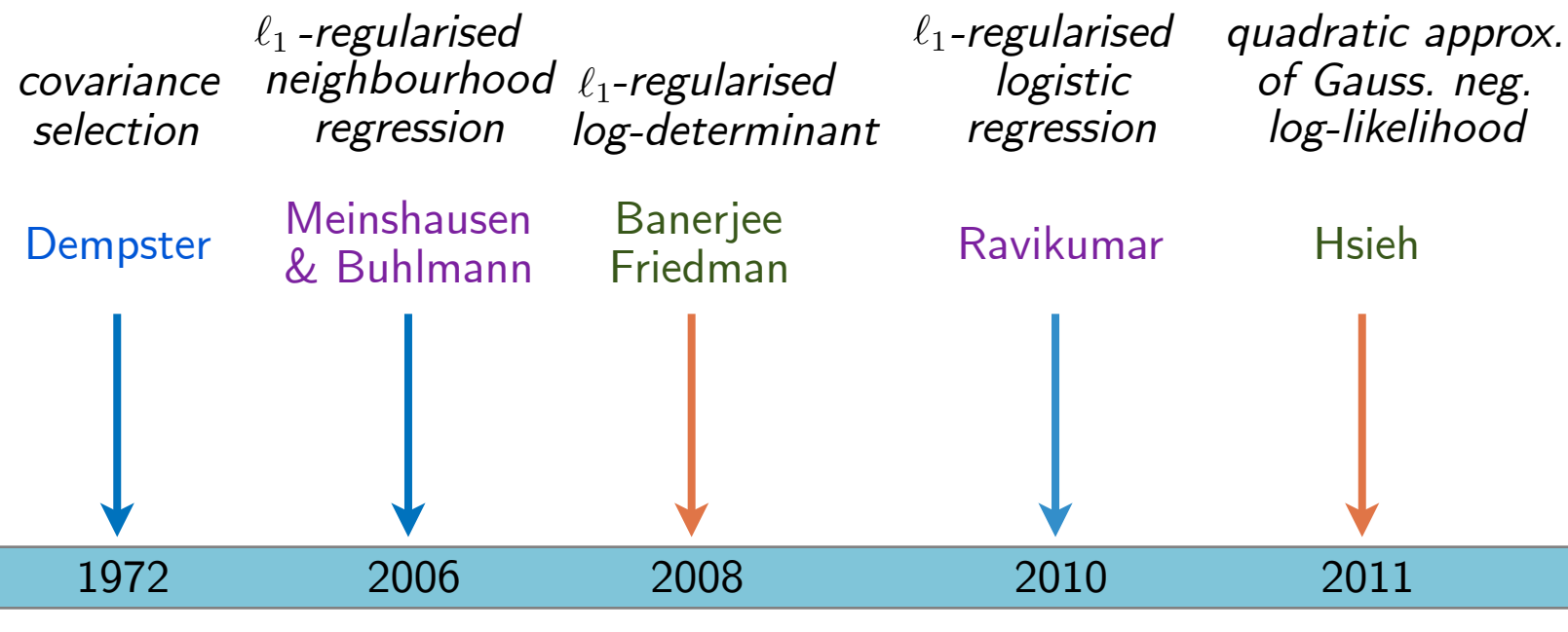
\mathbf{S}

graphical Lasso maximises likelihood of precision matrix Θ :

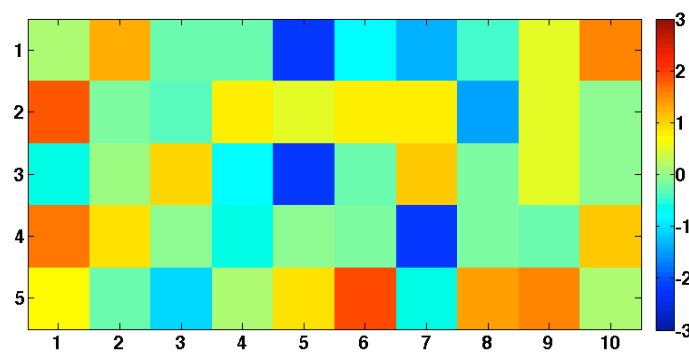
$$\max_{\Theta} \log \det \Theta - \text{tr}(\mathbf{S}\Theta) - \rho \|\Theta\|_1$$

log-likelihood function

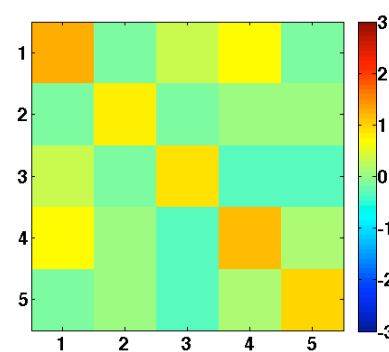
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 - learning graphs with non-negative weights?

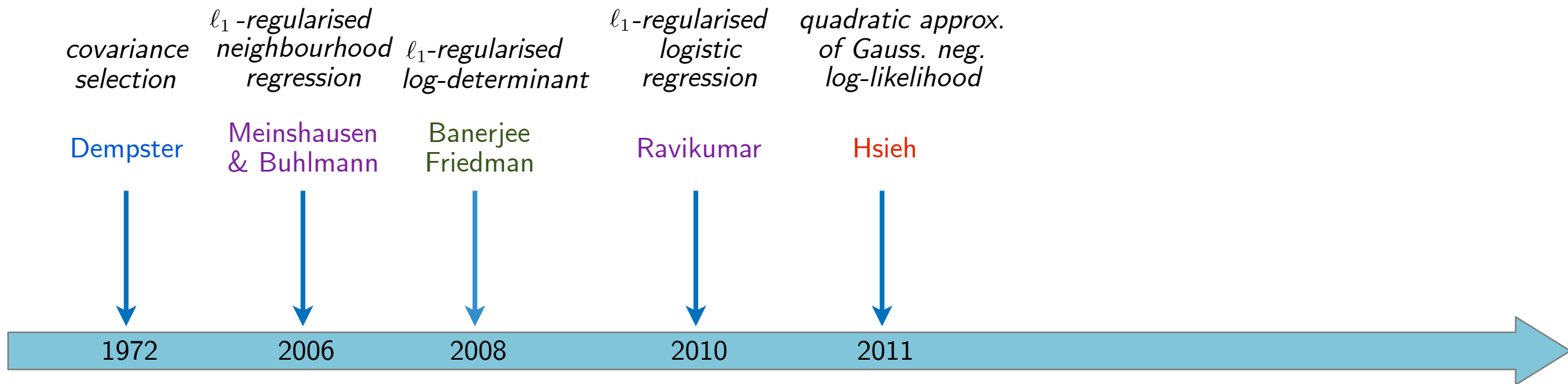
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 - M-matrices (symmetric, positive definite, non-positive off-diagonals) have been used as precision, leading to attractive GMRF [Slawski2015]
 - combinatorial **graph Laplacian L** belongs to M-matrices and is equivalent to graph topology

A (very partial) literature overview



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

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

from arbitrary precision matrix to graph Laplacian

A (very partial) literature overview

covariance selection ℓ_1 -regularised neighbourhood regression ℓ_1 -regularised log-determinant ℓ_1 -regularised logistic regression quadratic approx. of Gauss. neg. log-likelihood

Dempster

Meinshausen
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$$\text{s.t. } \Theta = \mathbf{L} + \frac{1}{\sigma^2} \mathbf{I}$$

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Lake

log-determinant
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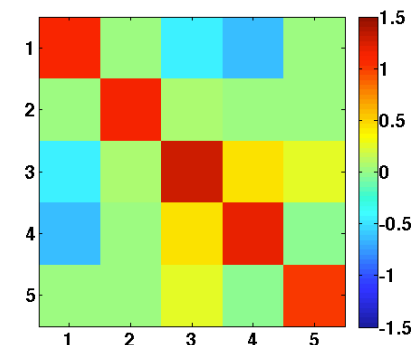
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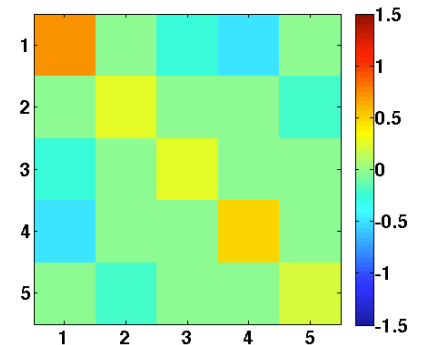
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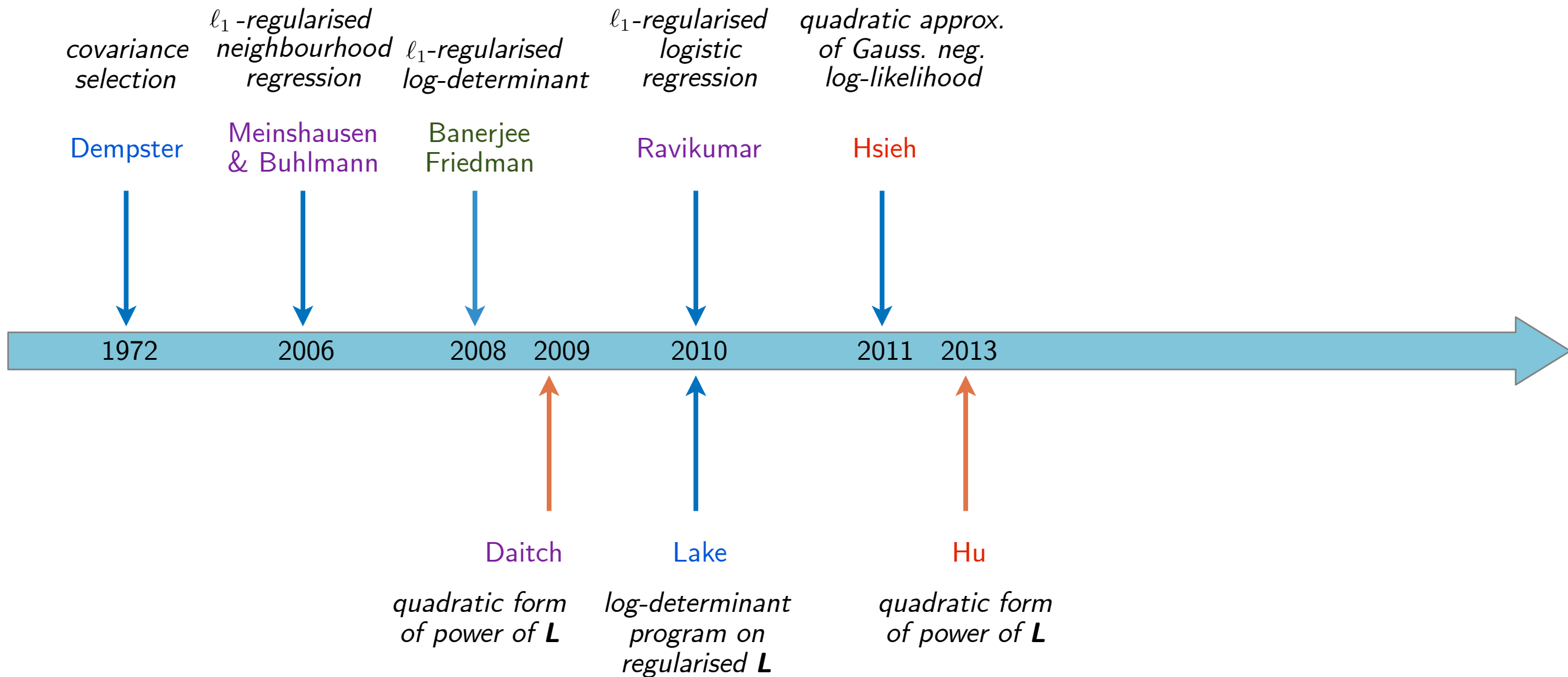
precision by
graphical Lasso



Laplacian by
Lake et al.

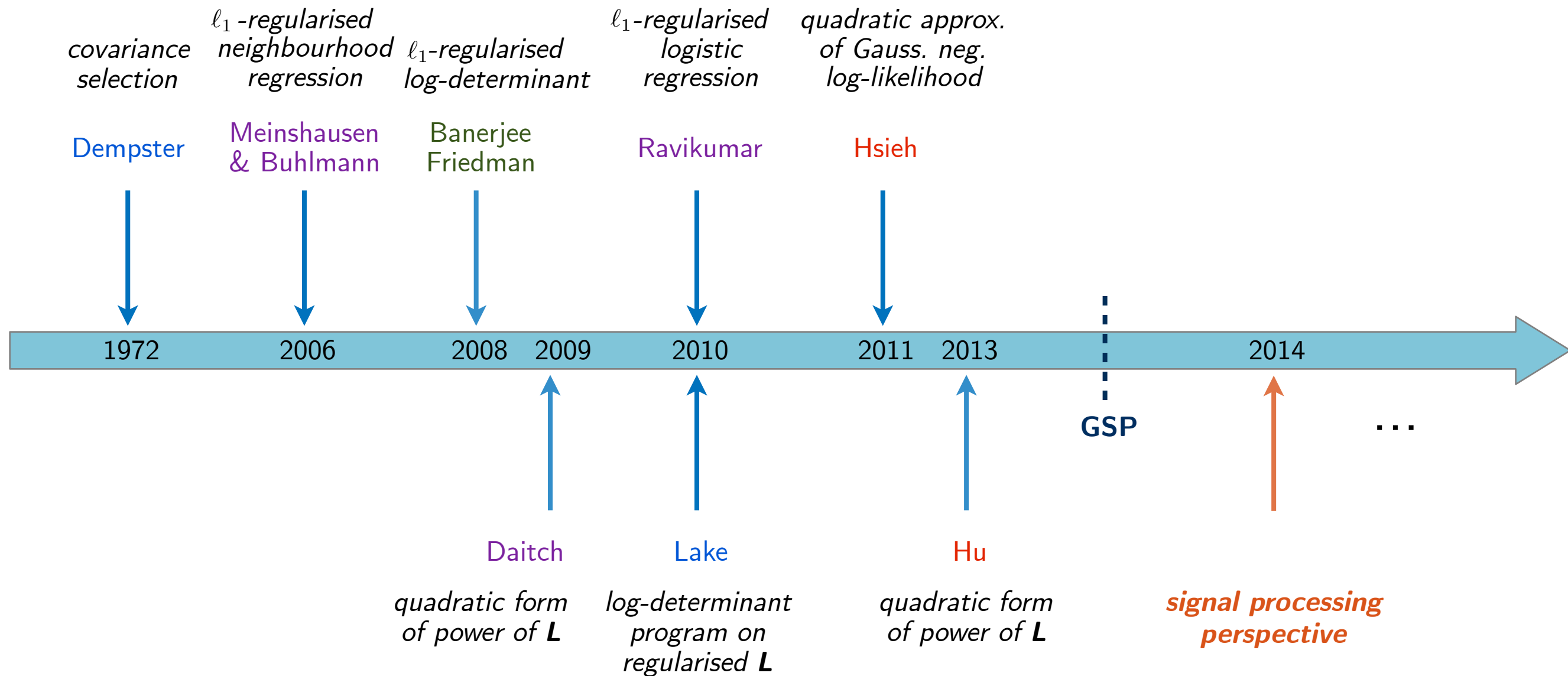
from arbitrary precision matrix to graph Laplacian

A (very partial) literature overview



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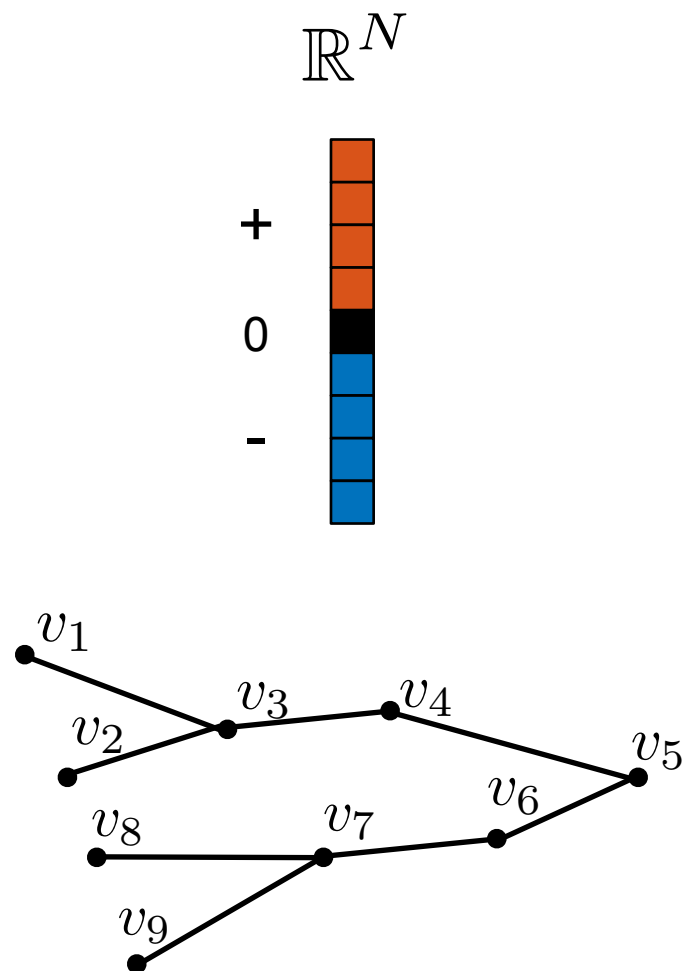
from arbitrary precision matrix to graph Laplacian
common setting in graph signal processing (GSP)

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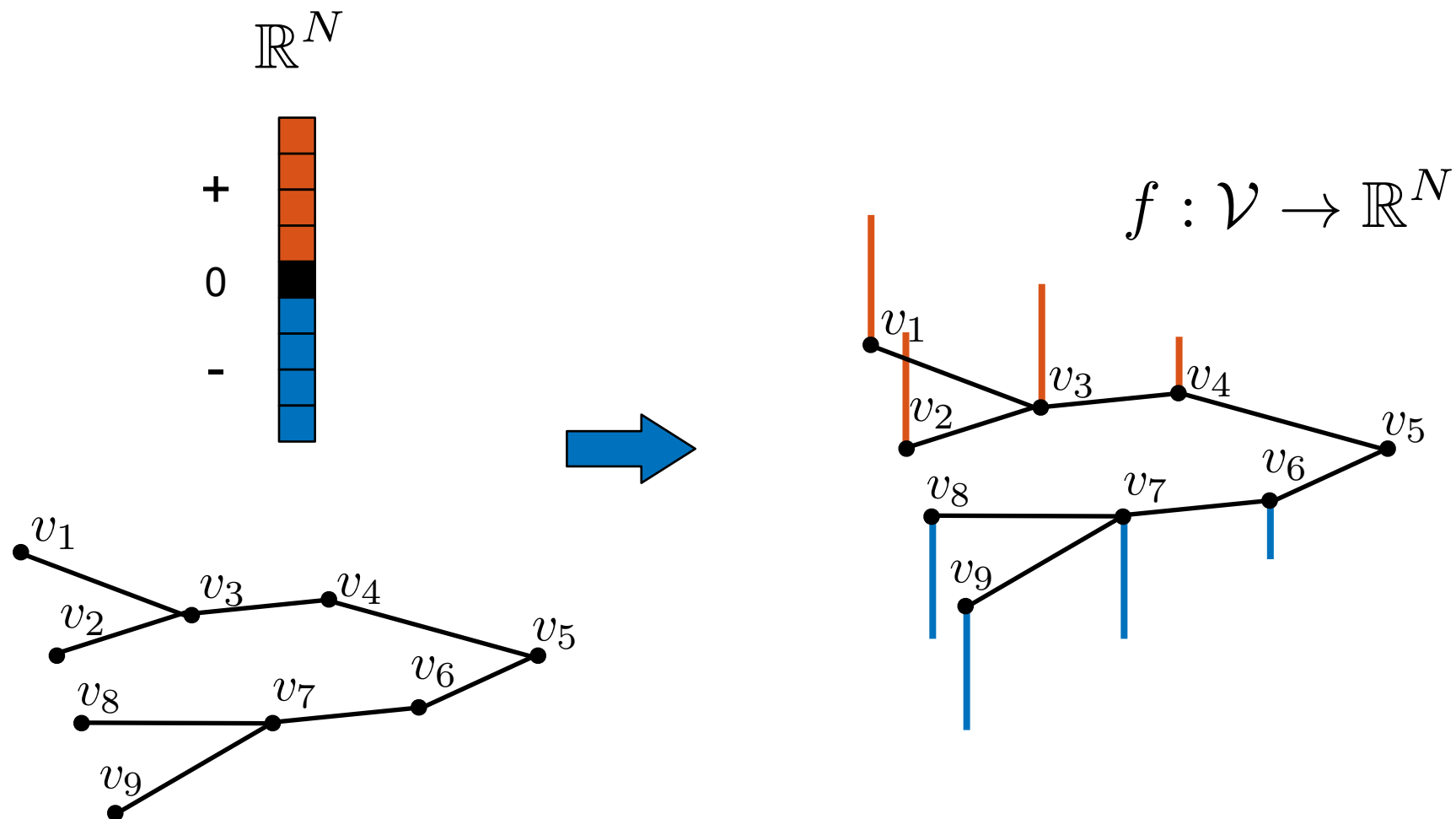
Graph signals

- Structured data can be represented by **graph signals**



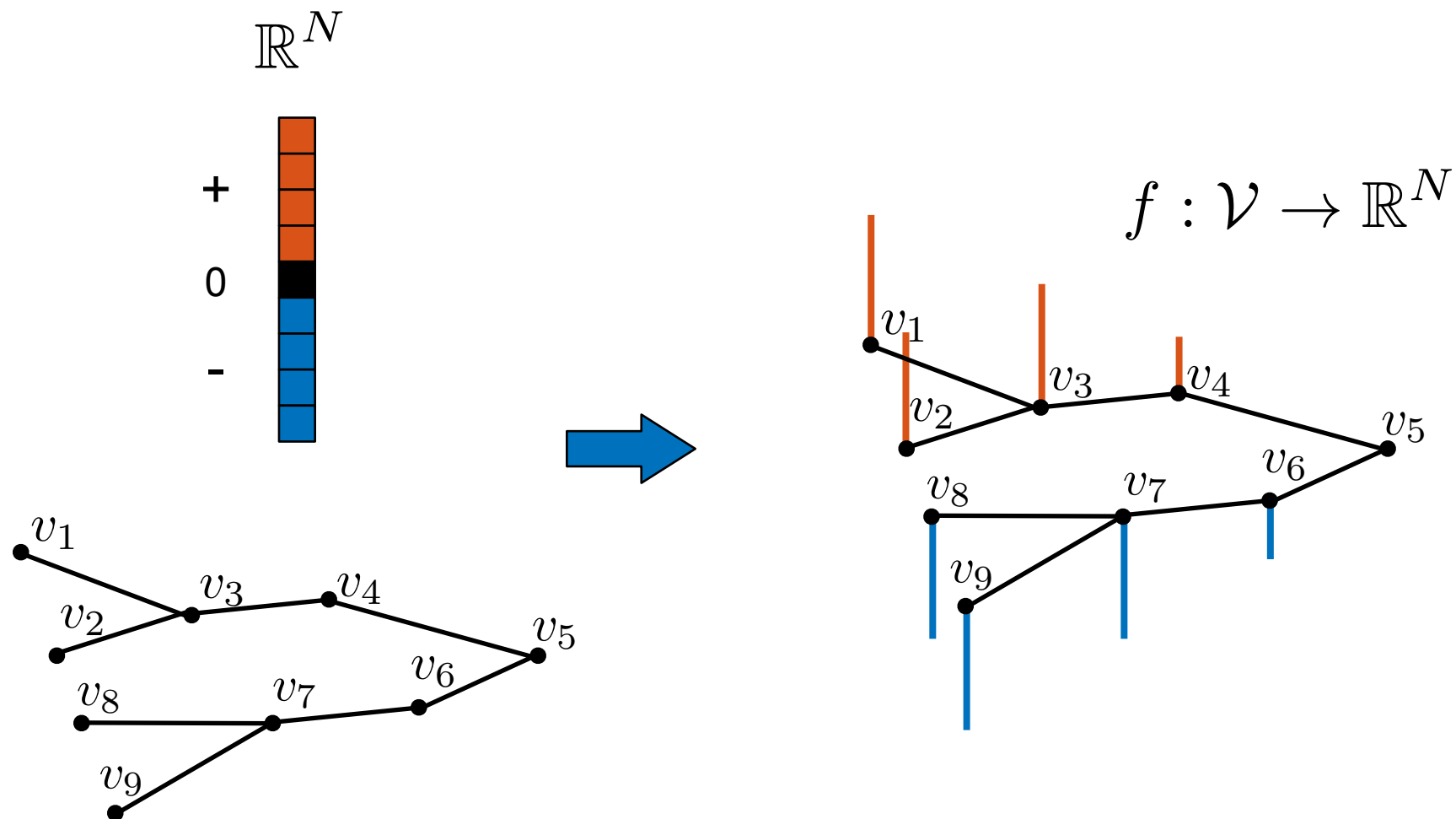
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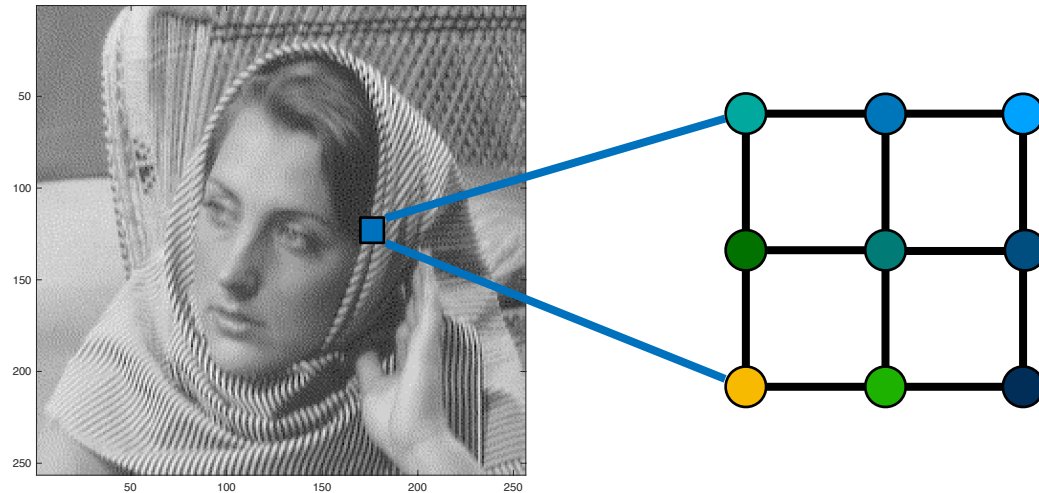
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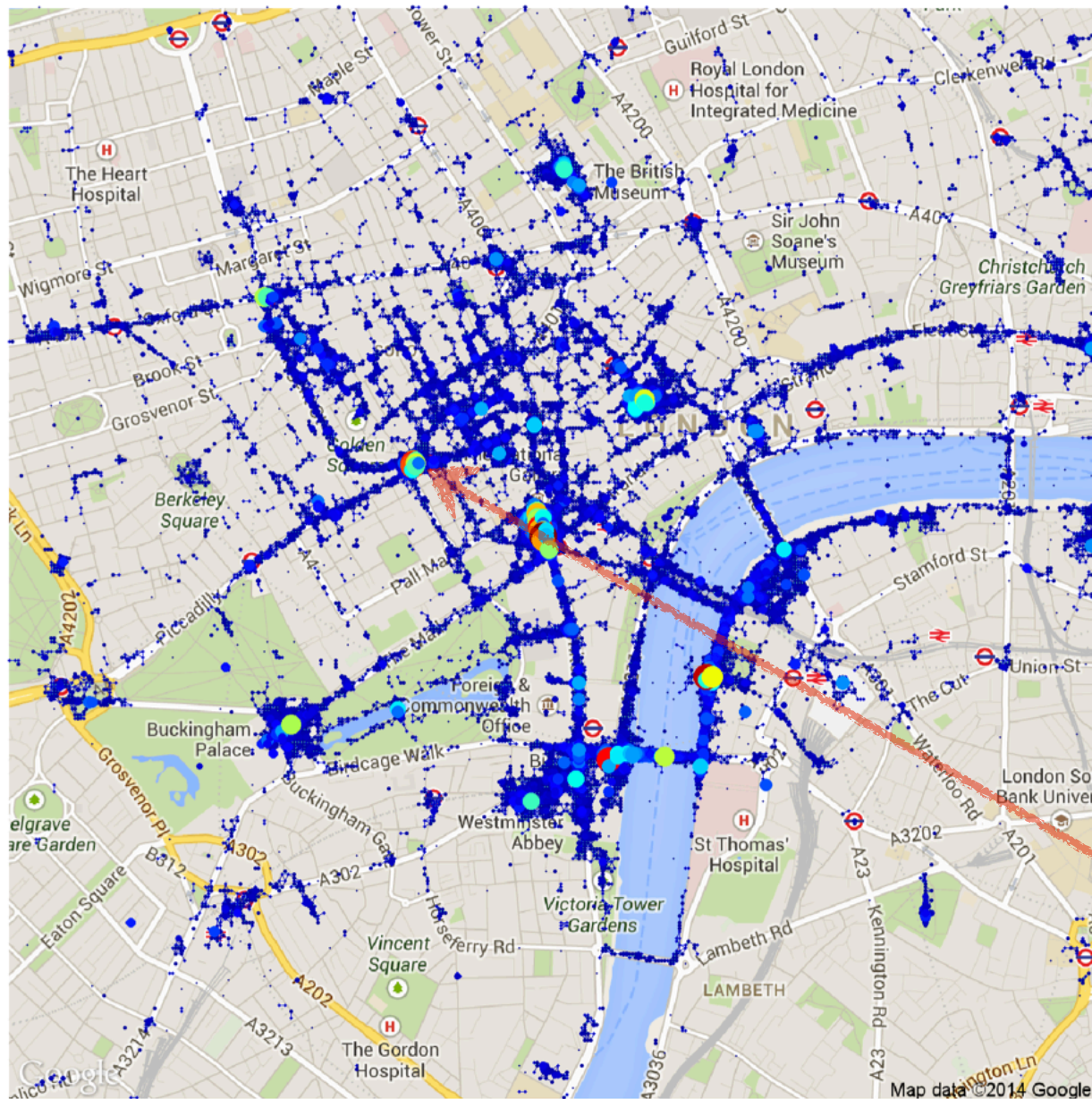
**takes into account both structure (edges) and
data (values at vertices)**

Graph signals are pervasive

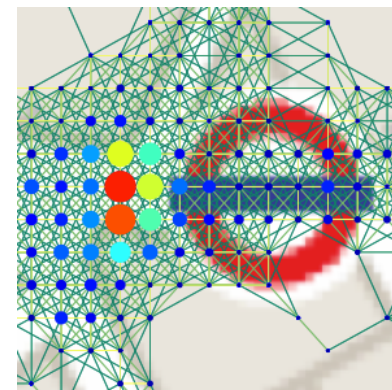


- Vertices:
 - regular grid
- Edges:
 - 4-nearest neighbour connection
- Signal:
 - pixel values

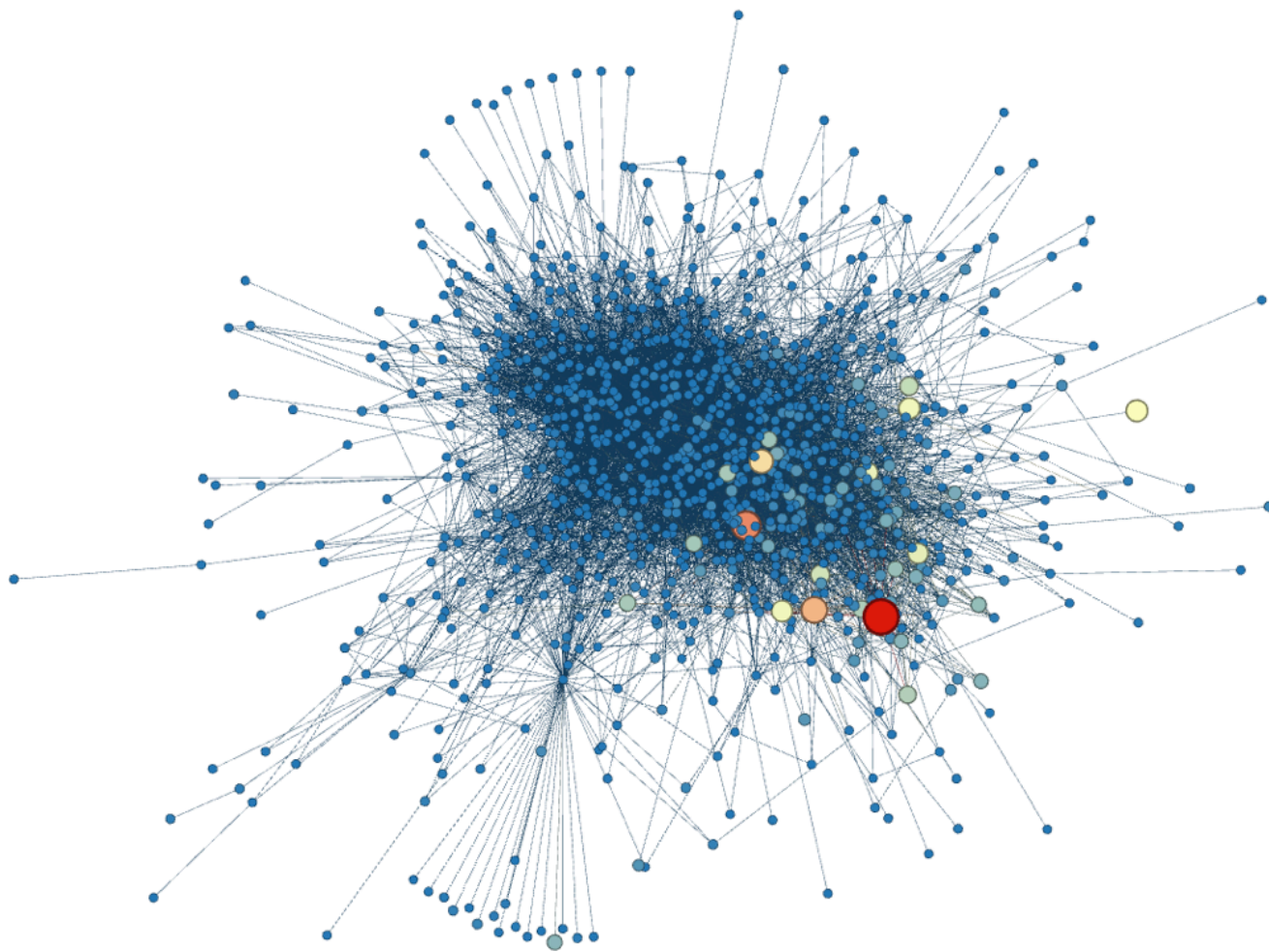
Graph signals are pervasive



- Vertices:
 - 9000 grid cells in London
- Edges:
 - geographical proximity of grid cells
- Signal:
 - # Flickr users who have taken photos in two and a half year

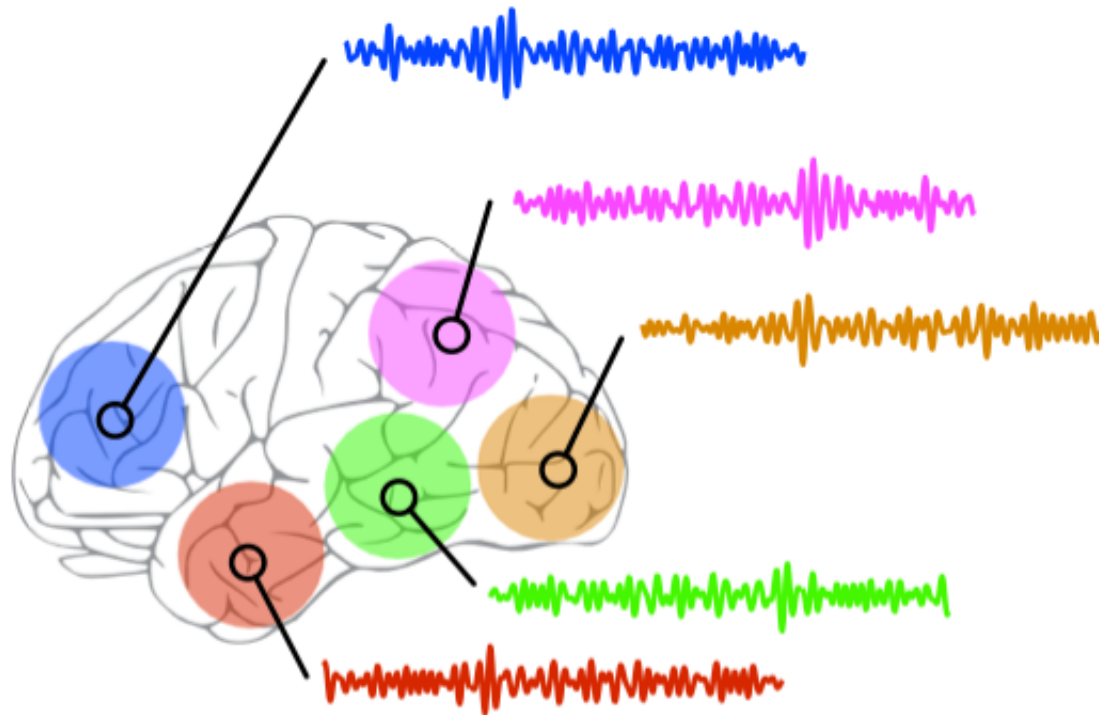


Graph signals are pervasive



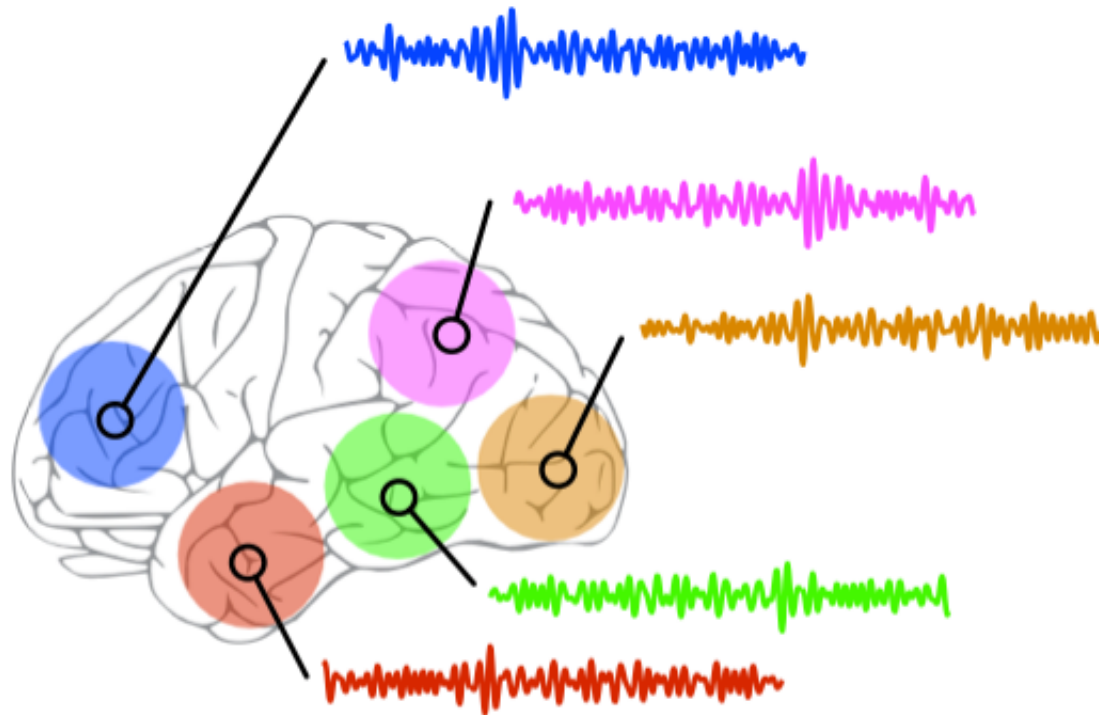
- Vertices:
 - 1000 Twitter users
- Edges:
 - following relationship among users
- Signal:
 - # Apple-related hashtags they have posted in six weeks

Graph signals are pervasive



- Vertices:
 - brain regions
- Edges:
 - structural connectivity (via diffusion spectrum imaging) between brain regions
- Signal:
 - blood-oxygen-level-dependent (BOLD) time series

Graph signals are pervasive

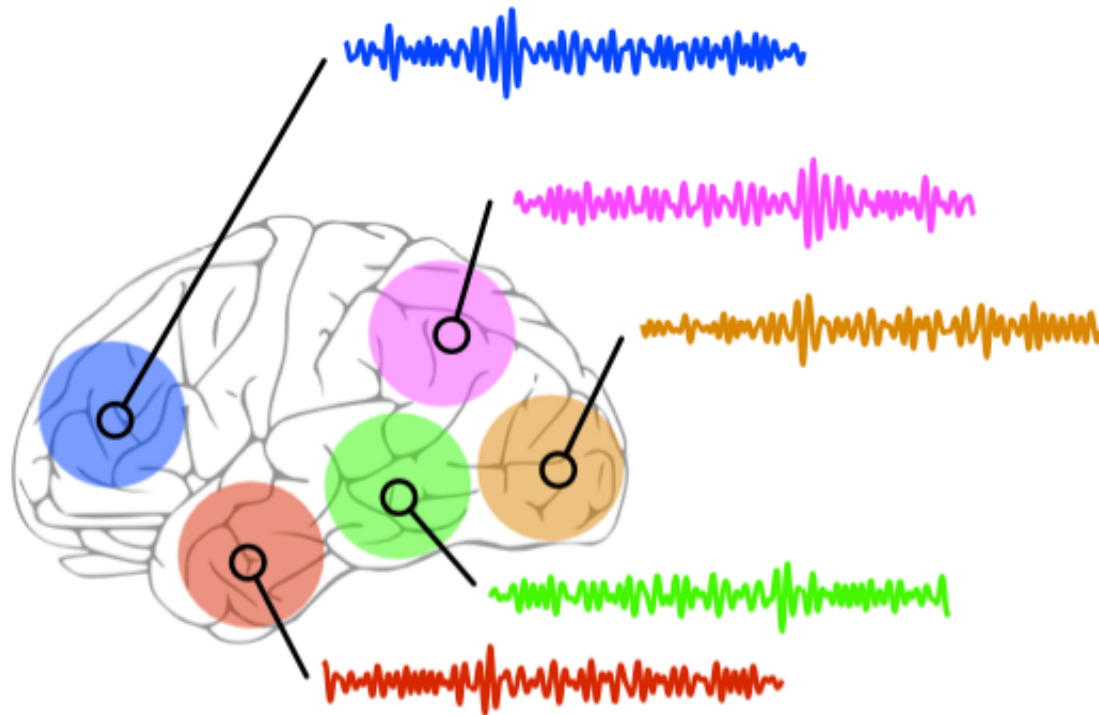


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how to generalise signal processing tools on graphs?

- notion of shift invariance?
- notion of frequency?

Graph signals are pervasive

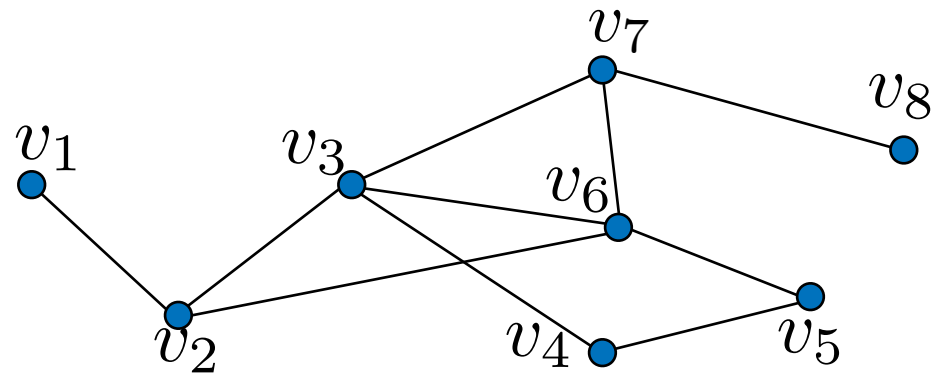


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how to generalise signal processing tools on graphs?

- notion of shift invariance? graph shift operator
- notion of frequency? graph Laplacian

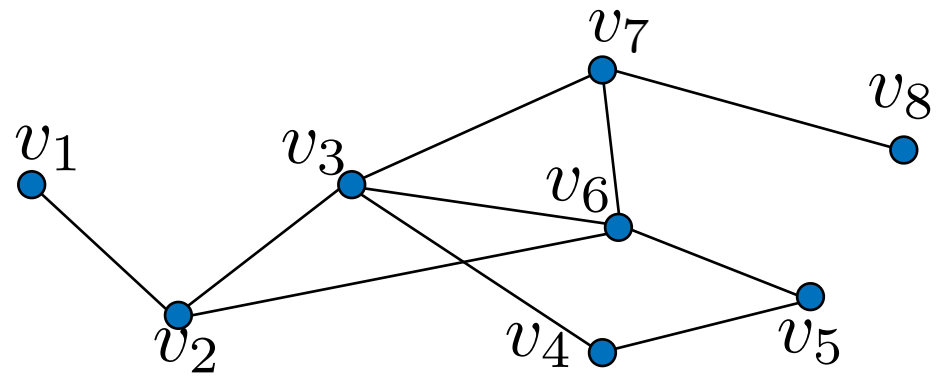
Graph Laplacian



Weighted and undirected graph:

$$\mathcal{G} = \{\mathcal{V}, \mathcal{E}\}$$

Graph Laplacian



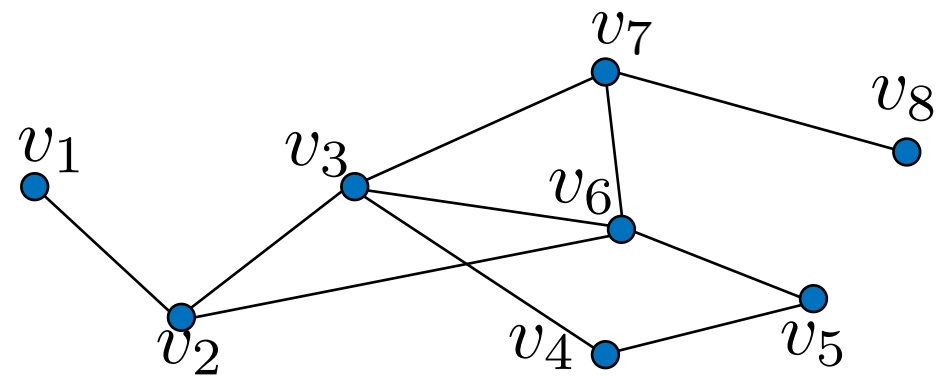
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$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

W

Graph Laplacian



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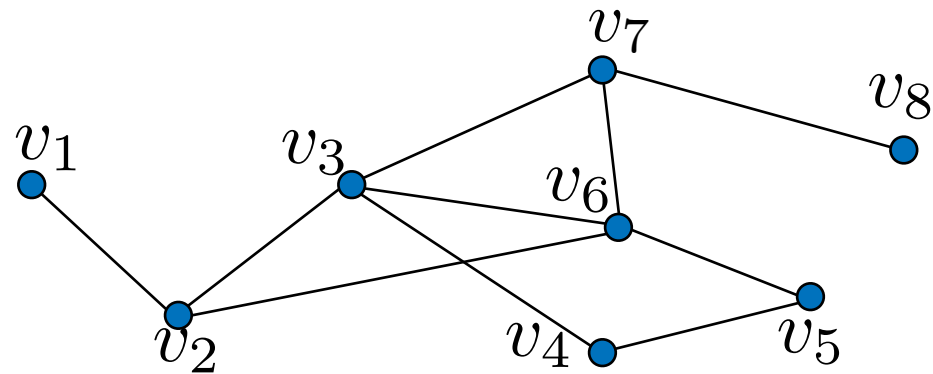
$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

D

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

W

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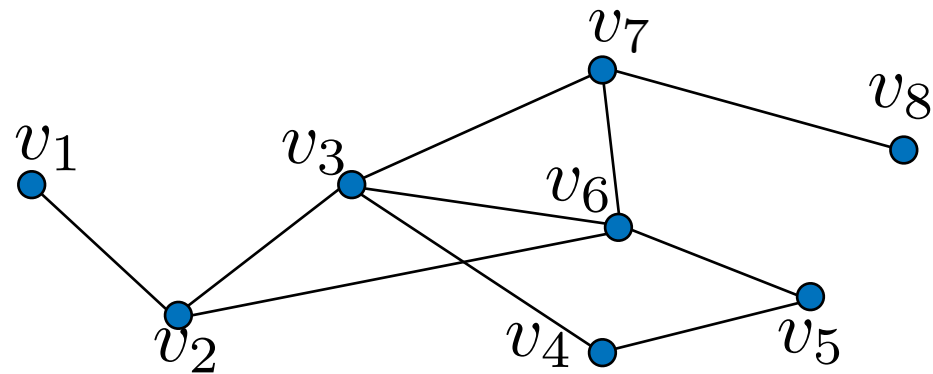
$$D = \text{diag}(d(v_1), \dots, d(v_N))$$

$$L = D - W \quad \textbf{Equivalent to G!}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 4 & -1 & 0 & -1 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & -1 & 0 & -1 & 4 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & -1 & 3 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

D
 W
 L

Graph Laplacian



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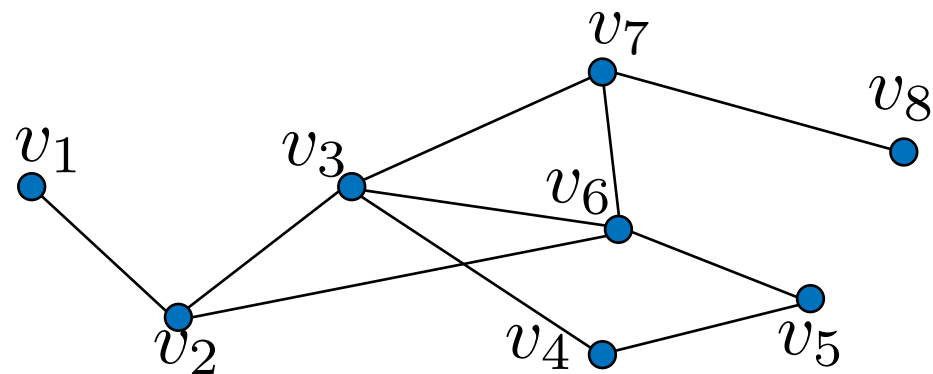
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$$L_{\text{norm}} = D^{-\frac{1}{2}} (D - W) D^{-\frac{1}{2}}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 4 & -1 & 0 & -1 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & -1 & 0 & -1 & 4 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & -1 & 3 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

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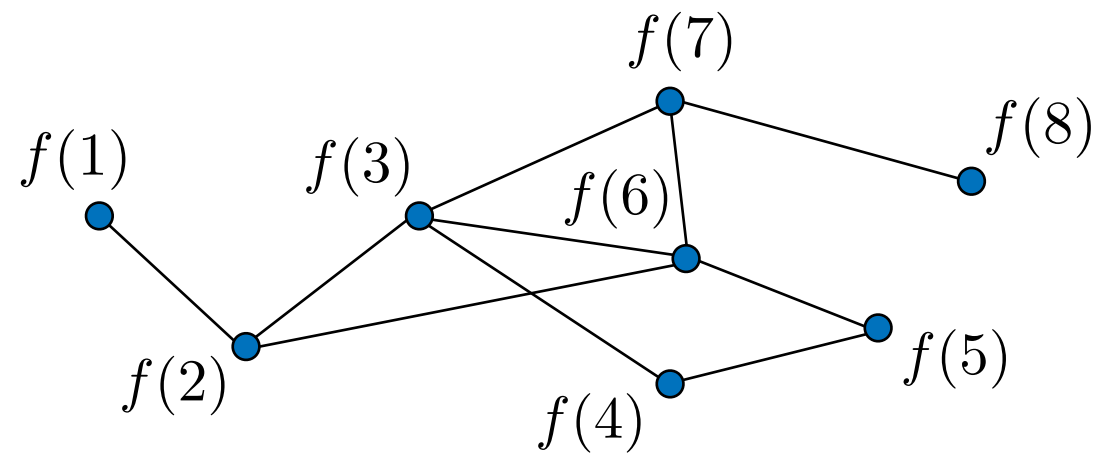
D
 W
 L

why graph Laplacian?

- standard stencil approximation of the Laplace operator
- provides a notion of “frequency” on graphs

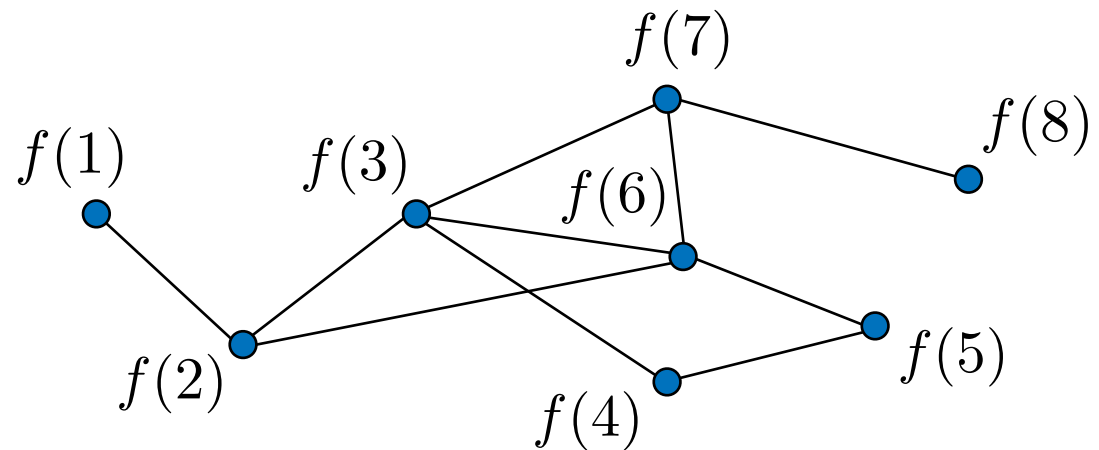
Graph Laplacian

$$f : \mathcal{V} \rightarrow \mathbb{R}^N$$



Graph Laplacian

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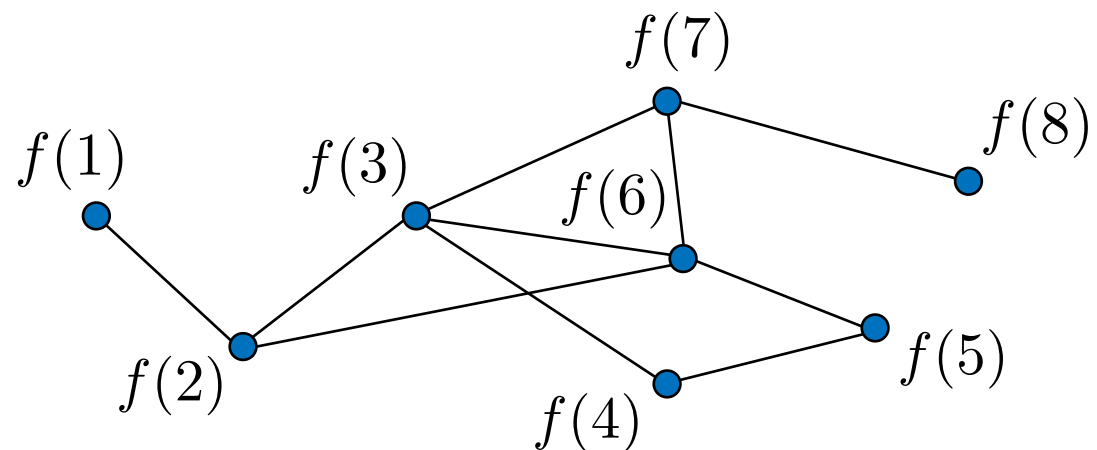


$$\begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 4 & -1 & 0 & -1 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & -1 & 0 & -1 & 4 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & -1 & 3 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} f(1) \\ f(2) \\ f(3) \\ f(4) \\ f(5) \\ f(6) \\ f(7) \\ f(8) \end{pmatrix}$$

$$Lf = \sum_{i,j=1}^N W_{ij} (f(i) - f(j))$$

Graph Laplacian

$$f : \mathcal{V} \rightarrow \mathbb{R}^N$$



$$\begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 4 & -1 & 0 & -1 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & -1 & 0 & -1 & 4 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & -1 & 3 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} f(1) \\ f(2) \\ f(3) \\ f(4) \\ f(5) \\ f(6) \\ f(7) \\ f(8) \end{pmatrix}$$

$$\begin{pmatrix} f(1) \\ f(2) \\ f(3) \\ f(4) \\ f(5) \\ f(6) \\ f(7) \\ f(8) \end{pmatrix}^T \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 4 & -1 & 0 & -1 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & -1 & 0 & -1 & 4 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & -1 & 3 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} f(1) \\ f(2) \\ f(3) \\ f(4) \\ f(5) \\ f(6) \\ f(7) \\ f(8) \end{pmatrix}$$

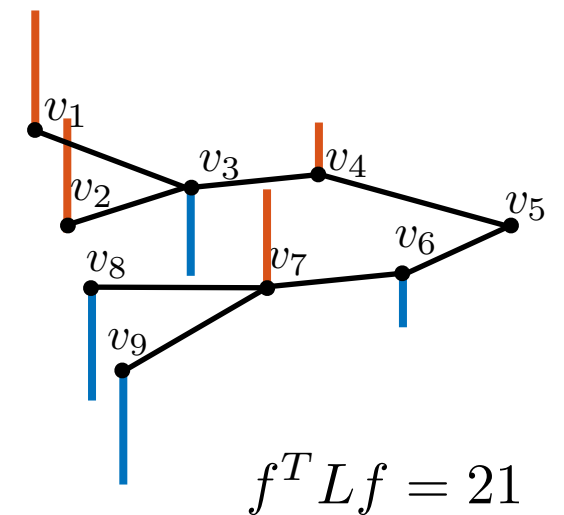
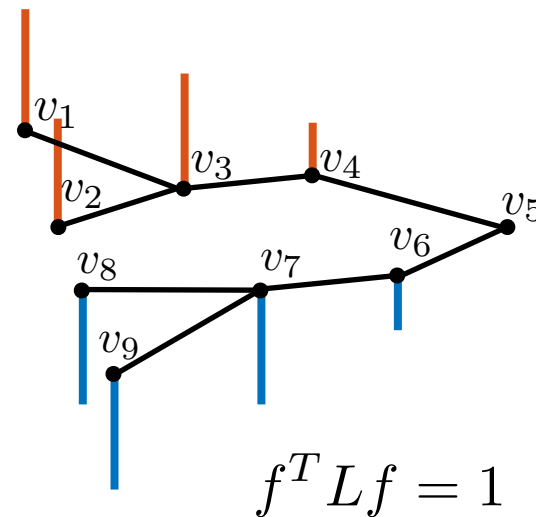
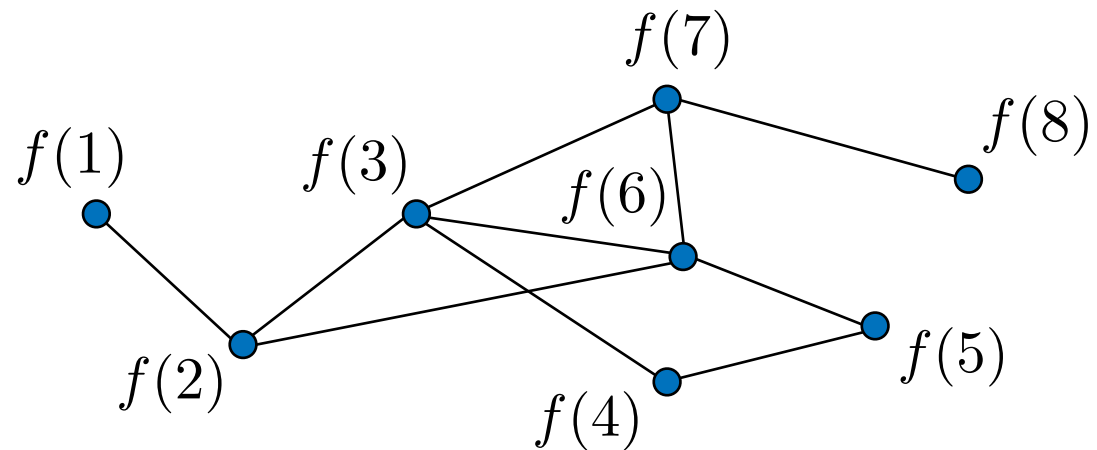
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$$f^T Lf = \frac{1}{2} \sum_{i,j=1}^N W_{ij} (f(i) - f(j))^2$$

measure of “smoothness” [Zhou04]

Graph Laplacian

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$$\begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 4 & -1 & 0 & -1 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & -1 & 0 & -1 & 4 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & -1 & 3 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} f(1) \\ f(2) \\ f(3) \\ f(4) \\ f(5) \\ f(6) \\ f(7) \\ f(8) \end{pmatrix}$$

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Graph Laplacian

- L has a complete set of orthonormal eigenvectors: $L = \chi \Lambda \chi^T$

$$L = \underbrace{\begin{bmatrix} | & & | \\ \chi_0 & \cdots & \chi_{N-1} \\ | & & | \end{bmatrix}}_{\chi} \underbrace{\begin{bmatrix} \lambda_0 & & 0 \\ & \ddots & \\ 0 & & \lambda_{N-1} \end{bmatrix}}_{\Lambda} \underbrace{\begin{bmatrix} \text{---} \chi_0 \text{---} \\ \cdots \\ \text{---} \chi_{N-1} \text{---} \end{bmatrix}}_{\chi^T}$$

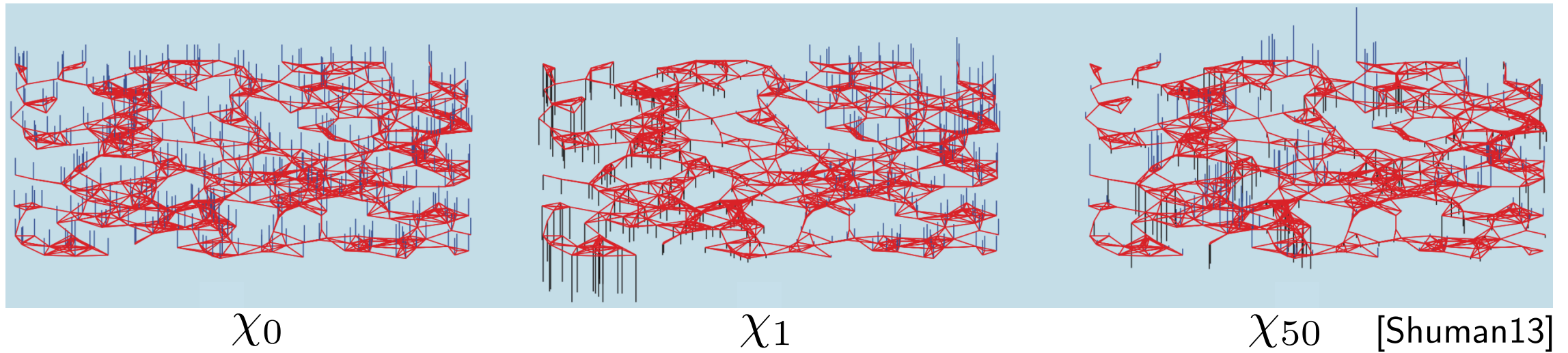
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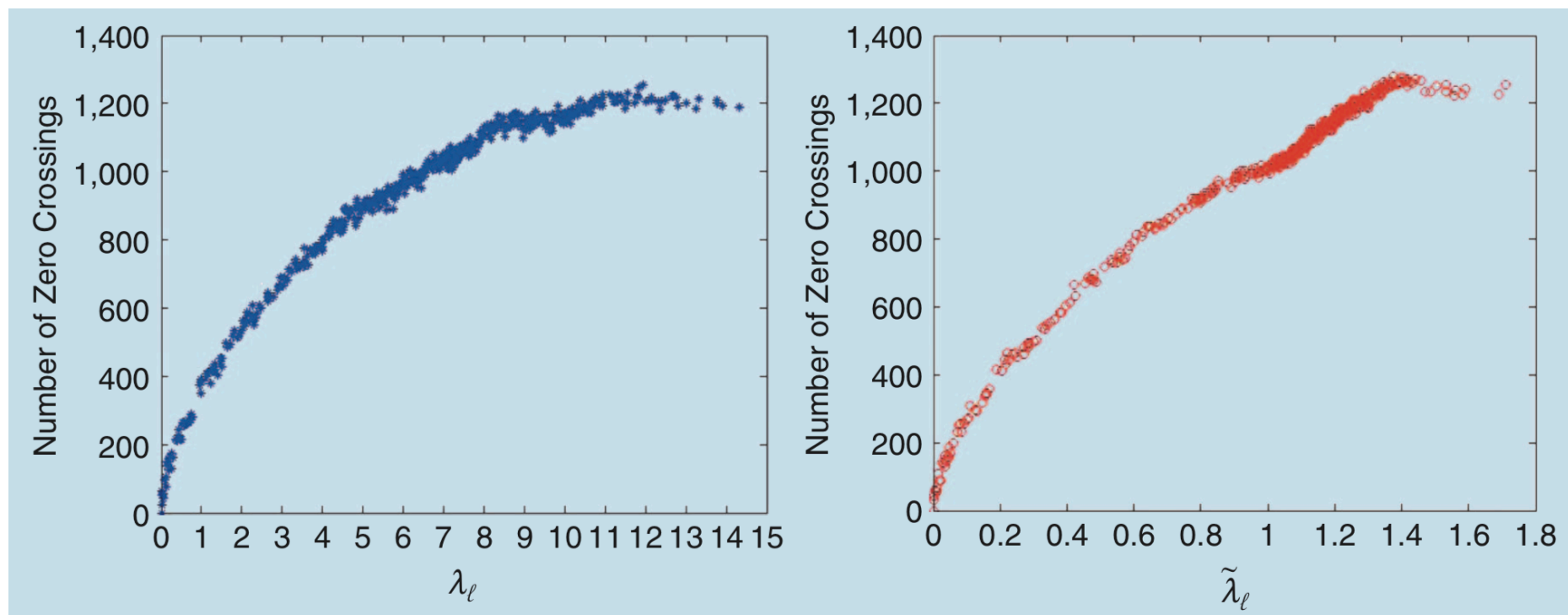
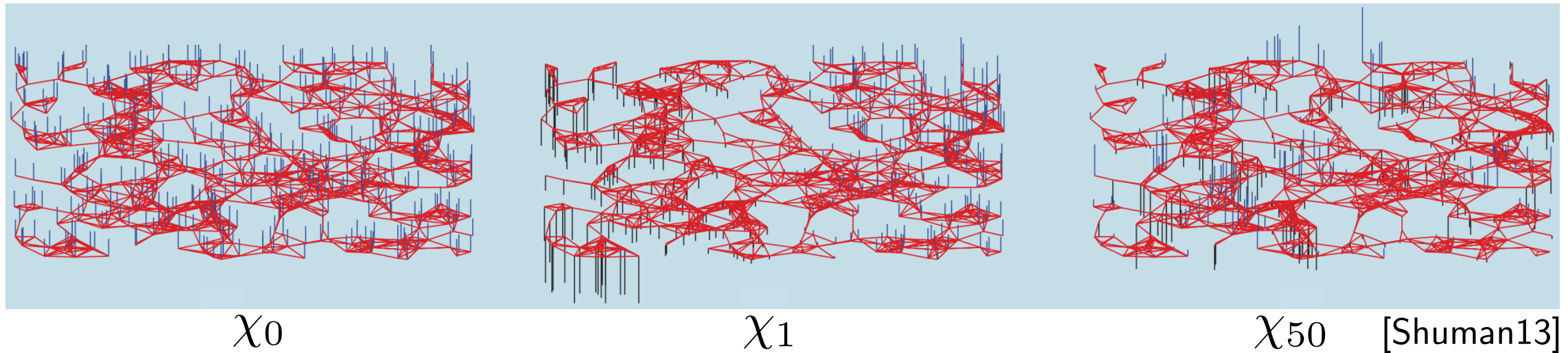
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- Eigenvalues are usually sorted increasingly: $0 = \lambda_0 < \lambda_1 \leq \dots \leq \lambda_{N-1}$

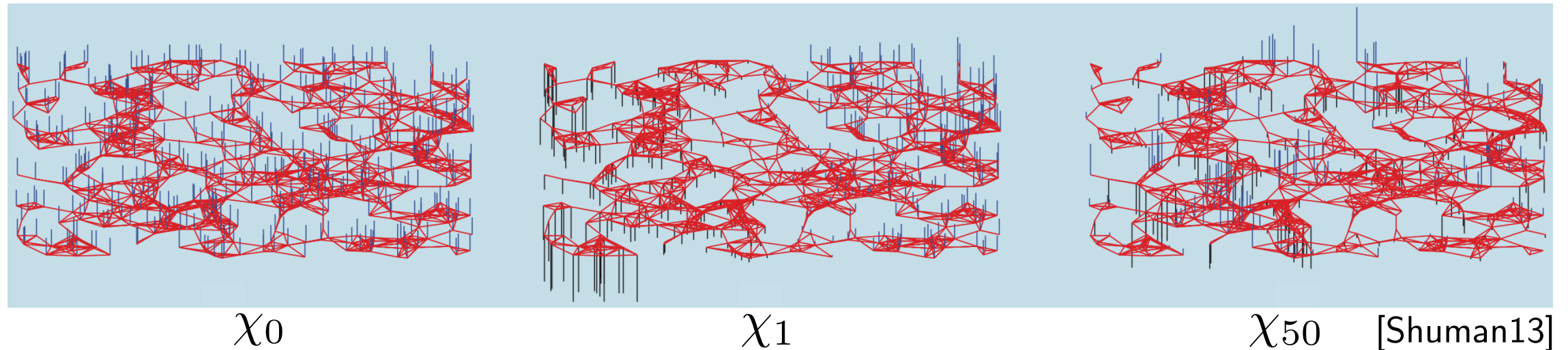
Graph Fourier transform



Graph Fourier transform



Graph Fourier transform



Low frequency

High frequency

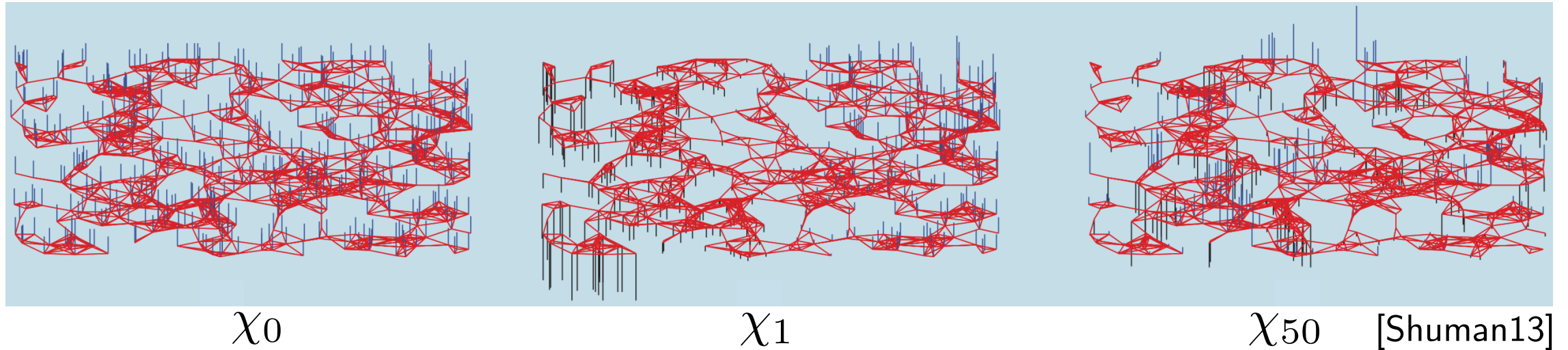
$$L = \chi \Lambda \chi^T$$

$$\chi_0^T L \chi_0 = \lambda_0 = 0$$

$$\chi_{50}^T L \chi_{50} = \lambda_{50}$$

- Eigenvectors associated with smaller eigenvalues have values that vary less rapidly along the edges

Graph Fourier transform



Low frequency

High frequency

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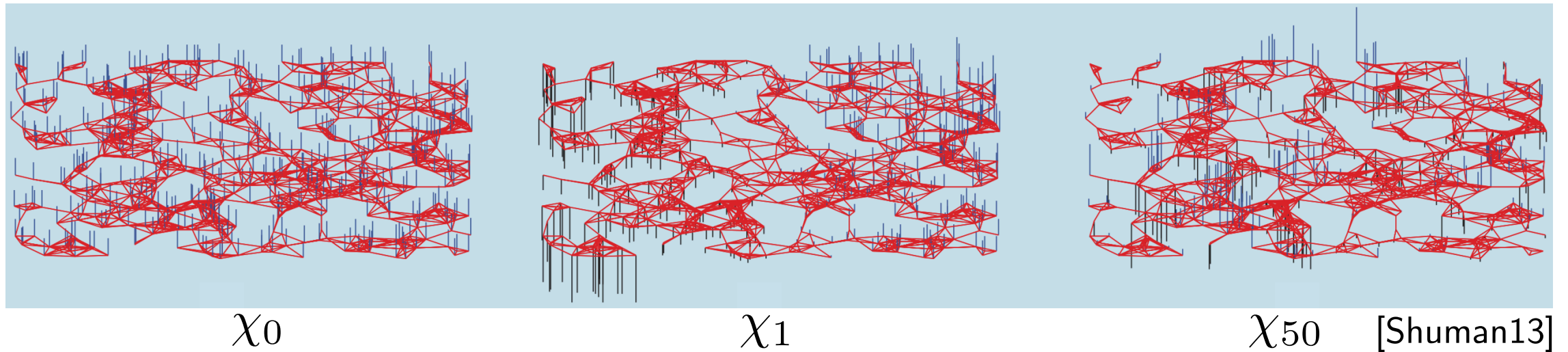
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Graph Fourier transform:
[Hammond11]

$$\hat{f}(\ell) = \langle \chi_\ell, f \rangle : \begin{bmatrix} | & & | \\ \chi_0 & \cdots & \chi_{N-1} \\ | & & | \end{bmatrix}^T \begin{bmatrix} | \\ f \\ | \end{bmatrix}$$

Graph Fourier transform



Low frequency

High frequency

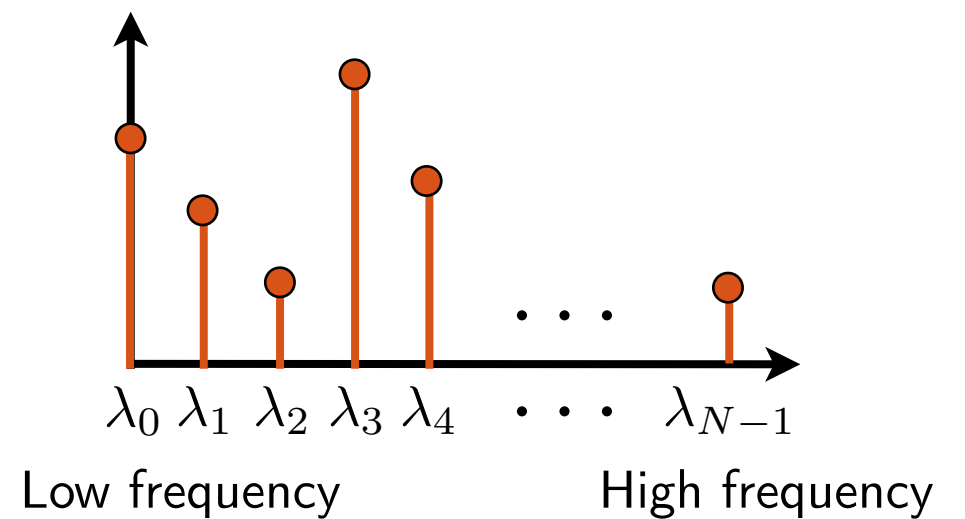
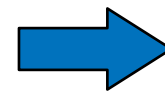
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Graph Fourier transform

- Laplacian L admits the following eigendecomposition: $L\chi_\ell = \lambda_\ell\chi_\ell$

Graph Fourier transform

- Laplacian L admits the following eigendecomposition: $L\chi_\ell = \lambda_\ell\chi_\ell$

one-dimensional Laplace operator: $-\nabla^2$



eigenfunctions: $e^{j\omega x}$



classical FT: $\hat{f}(\omega) = \int (e^{j\omega x})^* f(x) dx$

$$f(x) = \frac{1}{2\pi} \int \hat{f}(\omega) e^{j\omega x} d\omega$$

Graph Fourier transform

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graph Laplacian: L



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$f : V \rightarrow \mathbb{R}^N$

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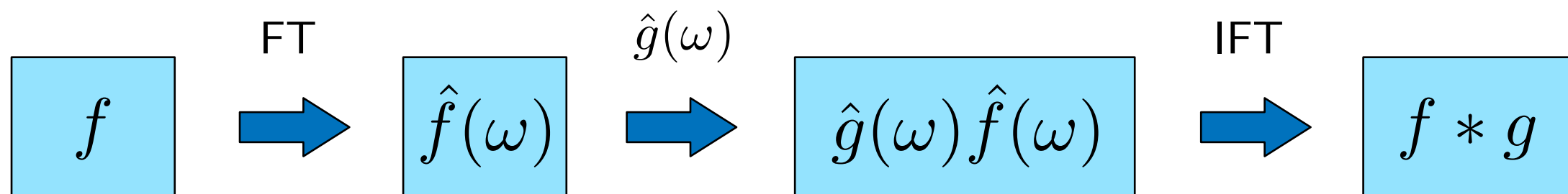
Classical frequency filtering

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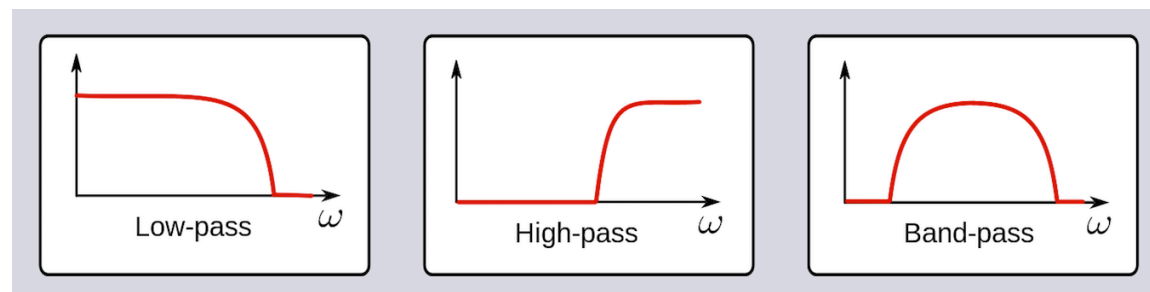
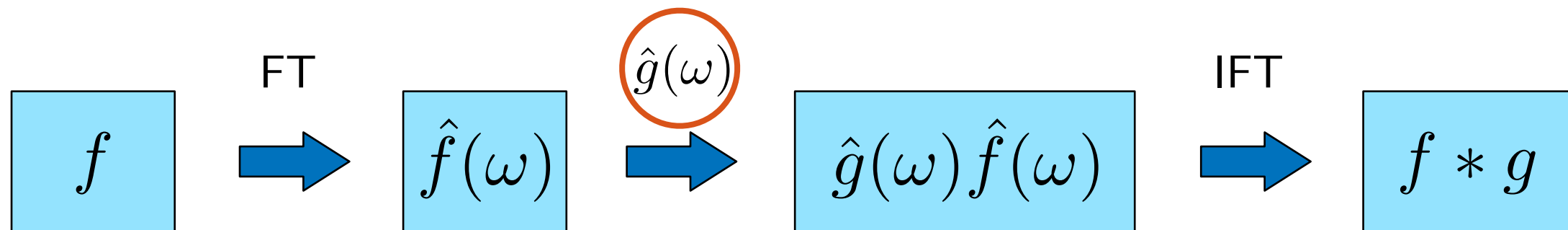
apply filter with transfer function $\hat{g}(\cdot)$ to a signal f



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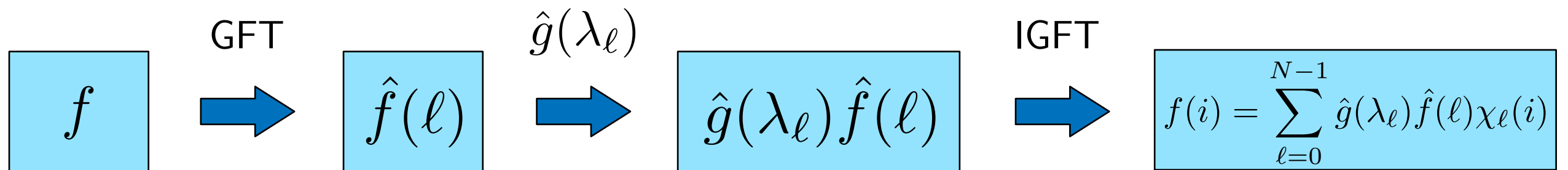
Graph spectral filtering

$$\text{GFT: } \hat{f}(\ell) = \langle \chi_\ell, f \rangle = \sum_{i=1}^N \chi_\ell^*(i) f(i) \quad f(i) = \sum_{\ell=0}^{N-1} \hat{f}(\ell) \chi_\ell(i)$$

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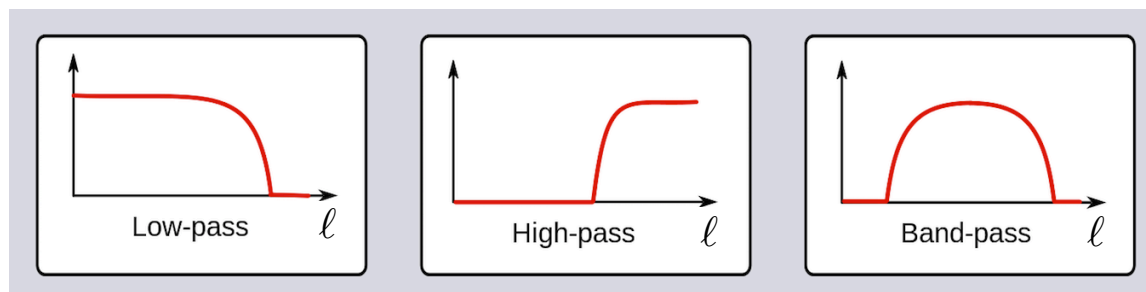
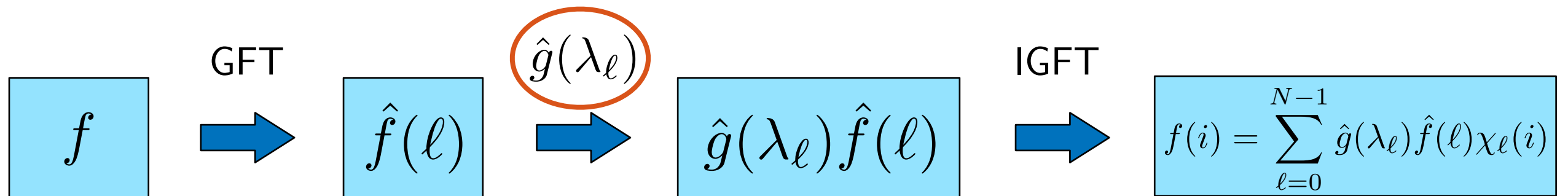
apply filter with transfer function $\hat{g}(\cdot)$ to a graph signal $f : \mathcal{V} \rightarrow \mathbb{R}^N$



Graph spectral filtering

$$\text{GFT: } \hat{f}(\ell) = \langle \chi_\ell, f \rangle = \sum_{i=1}^N \chi_\ell^*(i) f(i) \quad f(i) = \sum_{\ell=0}^{N-1} \hat{f}(\ell) \chi_\ell(i)$$

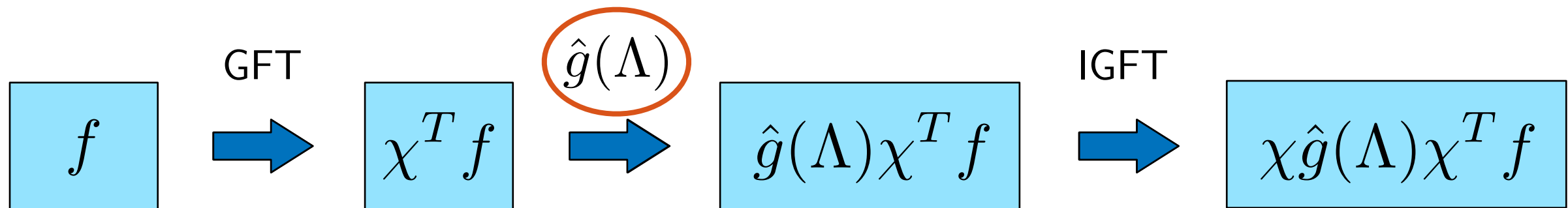
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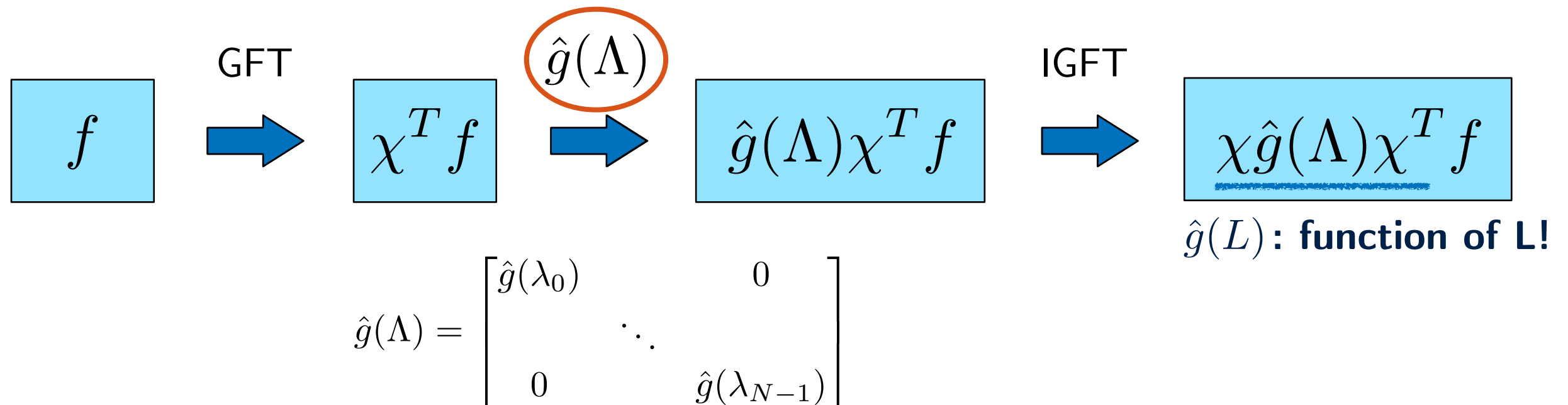


$$\hat{g}(\Lambda) = \begin{bmatrix} \hat{g}(\lambda_0) & & 0 \\ & \ddots & \\ 0 & & \hat{g}(\lambda_{N-1}) \end{bmatrix}$$

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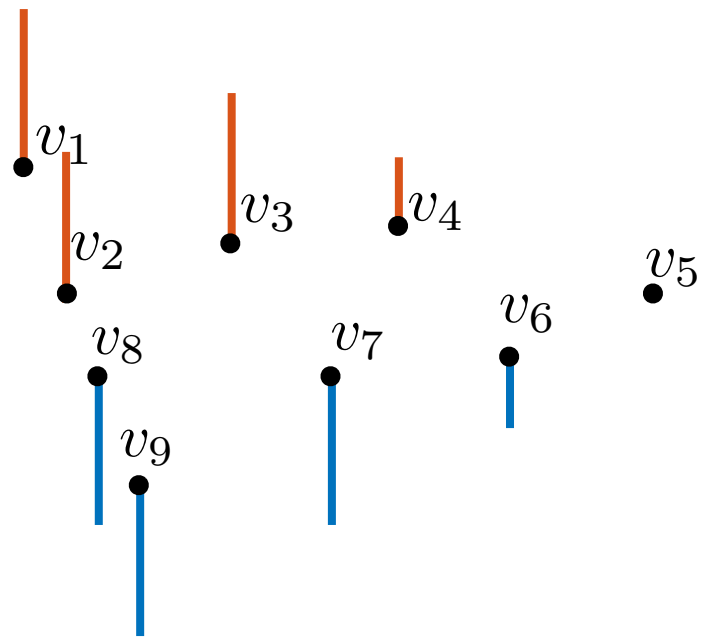
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Outline

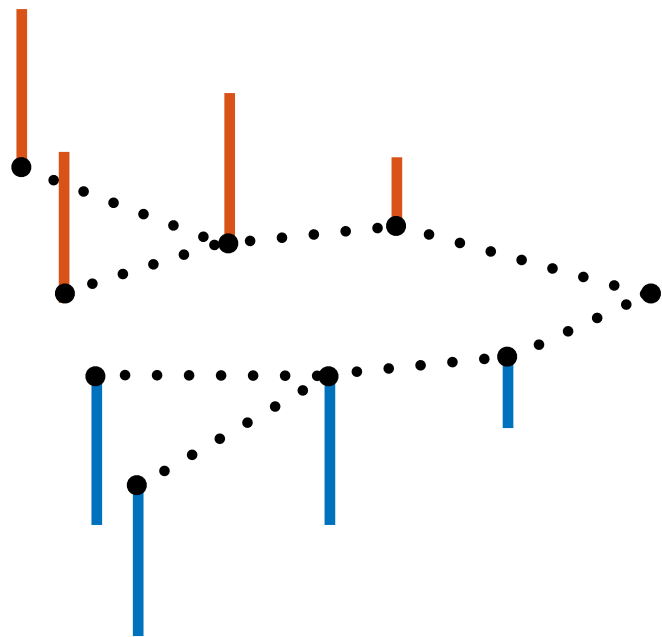
- A (very partial) literature overview
- A signal processing perspective
 - A brief introduction to graph signal processing (GSP)
 - GSP approaches for graph learning
- Concluding remarks

GSP for graph learning

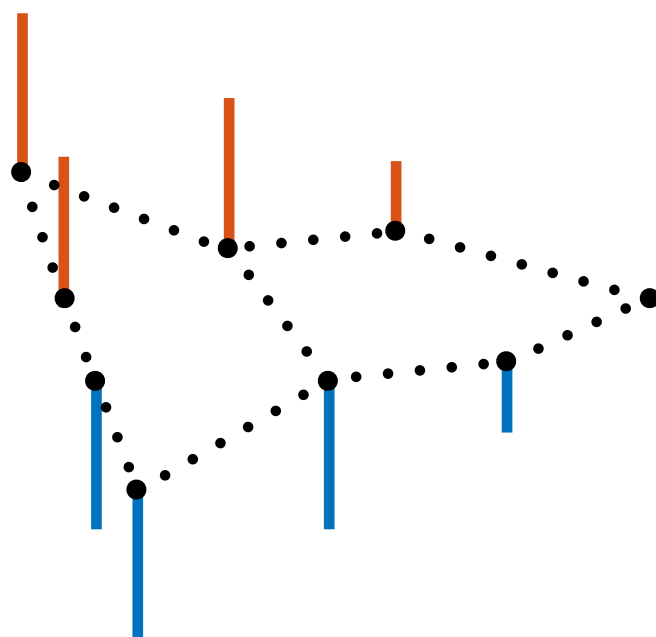


GSP for graph learning

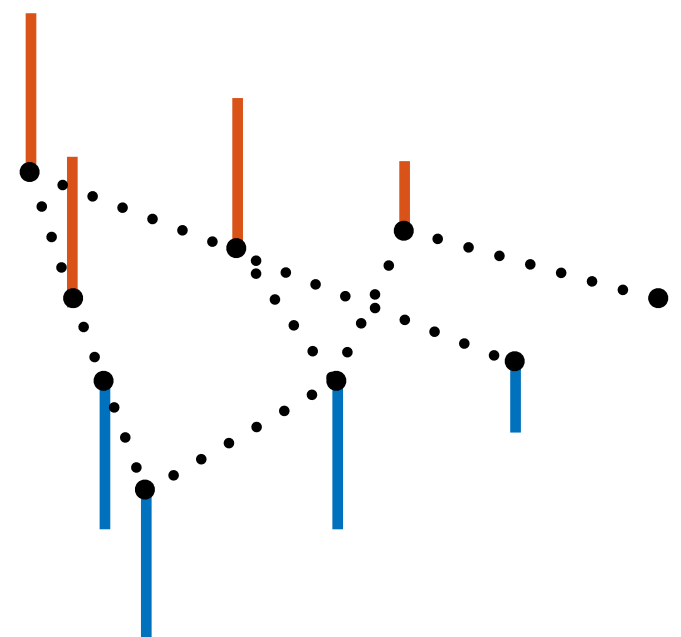
\mathcal{G}_1



\mathcal{G}_2

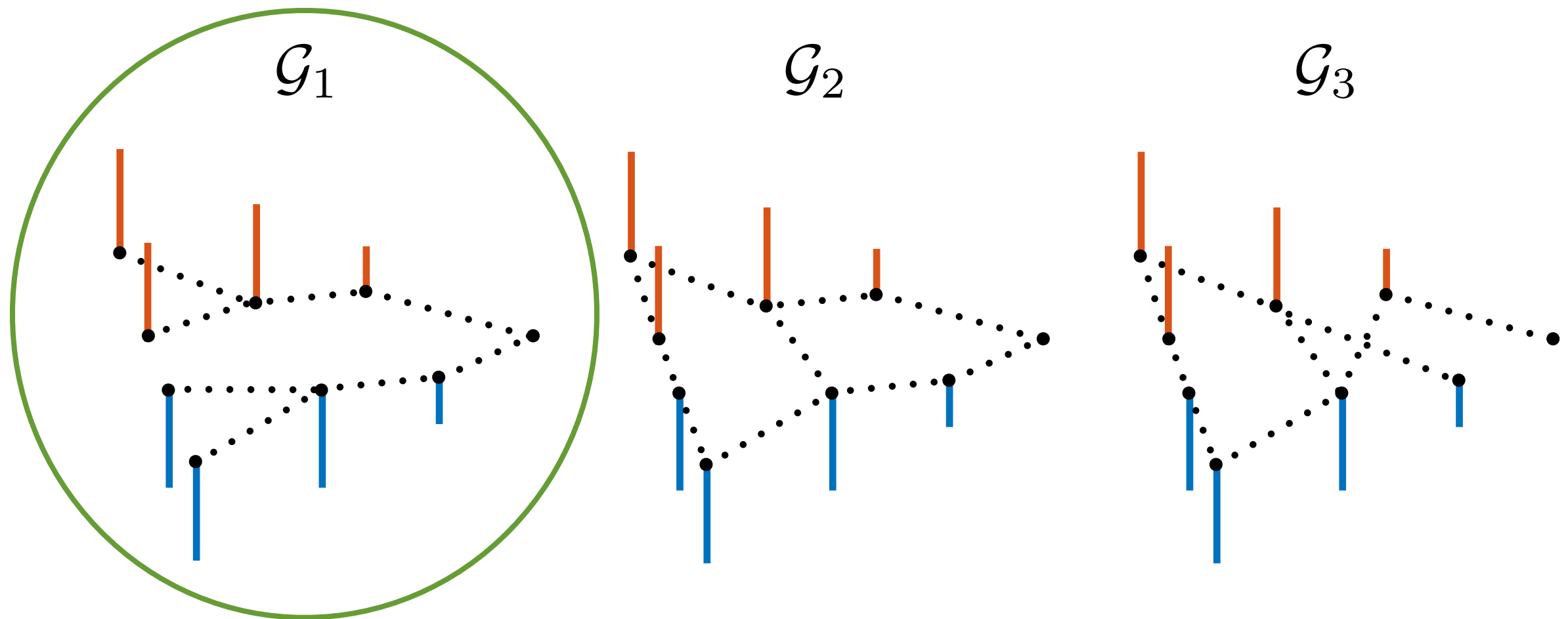


\mathcal{G}_3



which graph to choose?

GSP for graph learning



which graph to choose?

- depends on the signal/graph model
- idea: choose one that enforces certain signal characteristics

GSP for graph learning

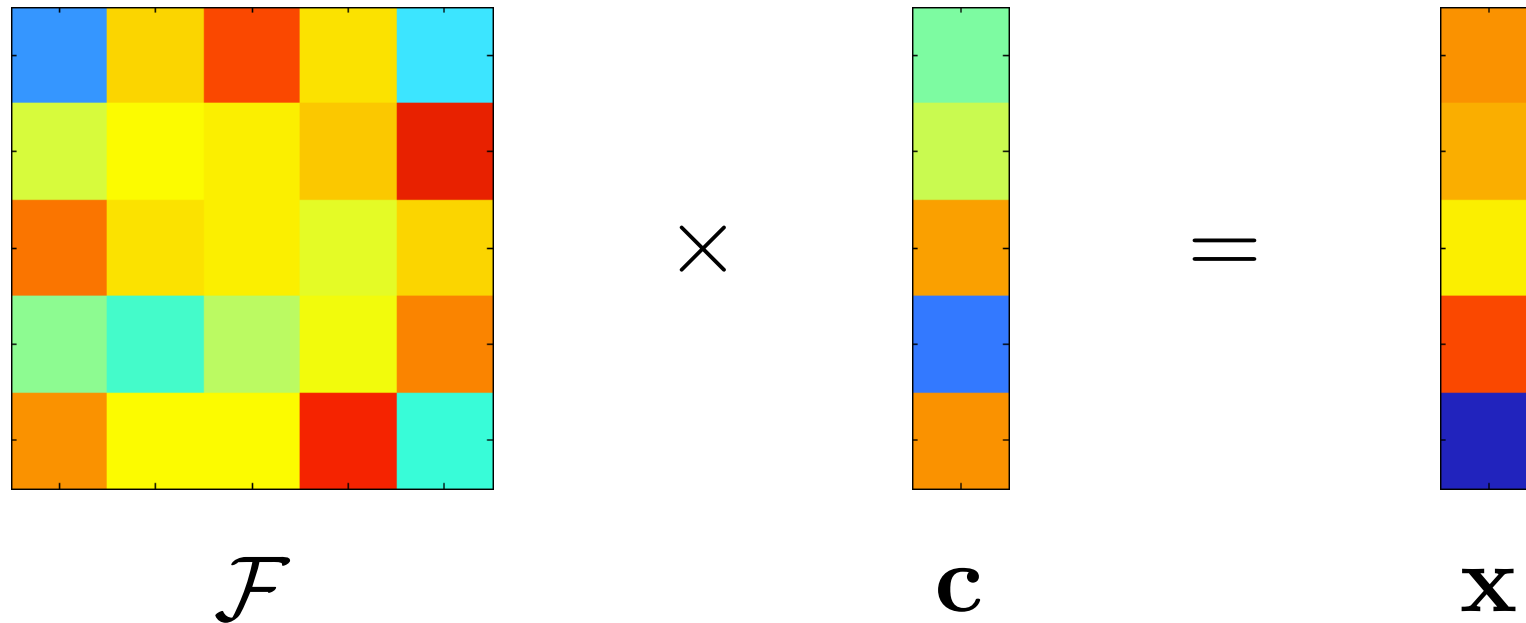
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GSP for graph learning

- Existing approaches have limitations
 - simple correlation or similarity function is not enough
 - statistical models do not always lead to non-negative edge weights
 - many impose a “global” distribution or behaviour
- Opportunity and challenge for GSP
 - GSP tools offer another “regulariser” for complicated inference: frequency or spectral representation
 - filtering-based approaches can provide generative models for signals with complex (non-Gaussian) behaviour

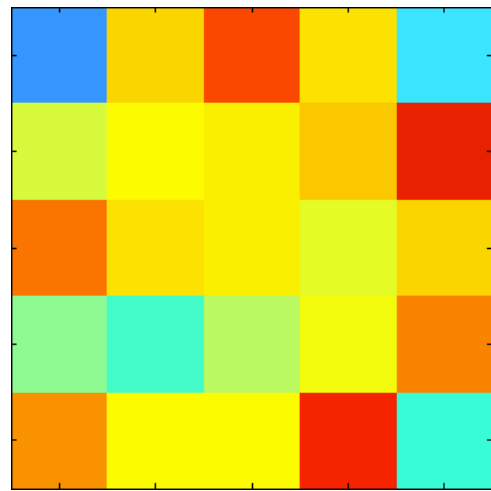
GSP for graph learning

- Signal processing is about $\mathbf{F} \mathbf{c} = \mathbf{x}$



GSP for graph learning

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



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

\times

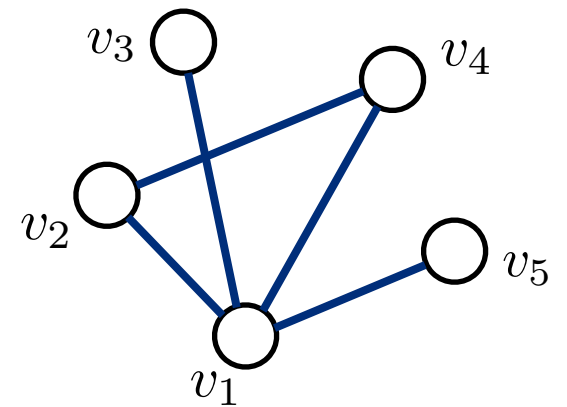


\mathbf{c}

$=$



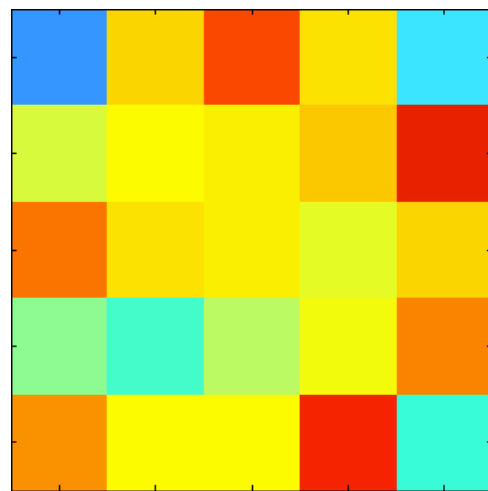
\mathbf{x}



\mathcal{G}

GSP for graph learning

- Forward: given \mathbf{G} and \mathbf{x} , design \mathbf{F} to study \mathbf{c}



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

Fourier/wavelet
atoms

trained dictionary
atoms

\times



\mathbf{c}

graph Fourier/
wavelet coefficient

graph dictionary
coefficient

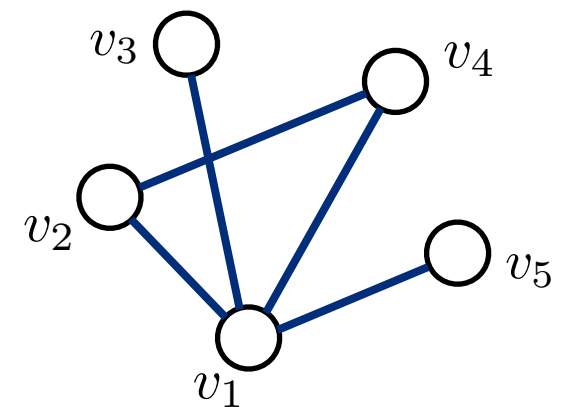
$=$



\mathbf{x}

[Coifman06,Narang09,Hammond11,
Shuman13,Sandryhaila13]

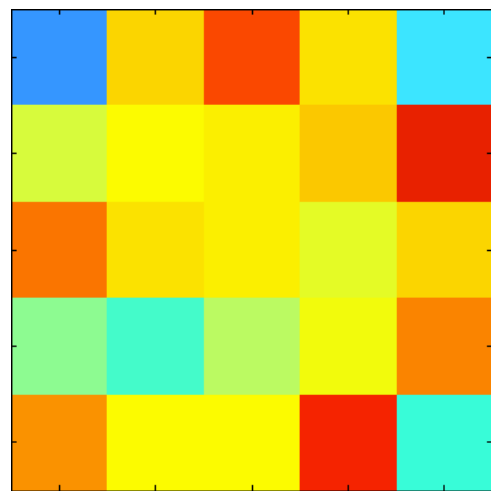
[Zhang12,Thanou14]



\mathcal{G}

GSP for graph learning

- Backward (graph learning): given \mathbf{x} , design \mathbf{F} and \mathbf{c} to infer \mathbf{G}



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

\times

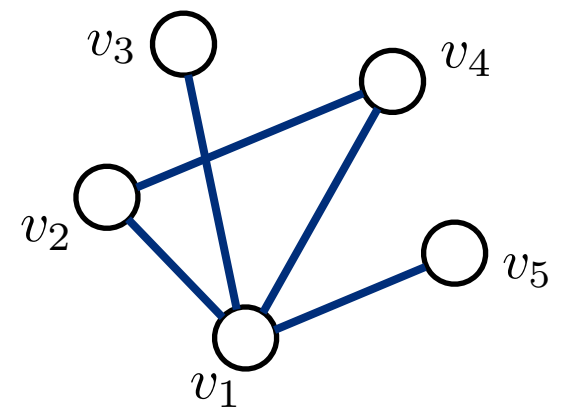


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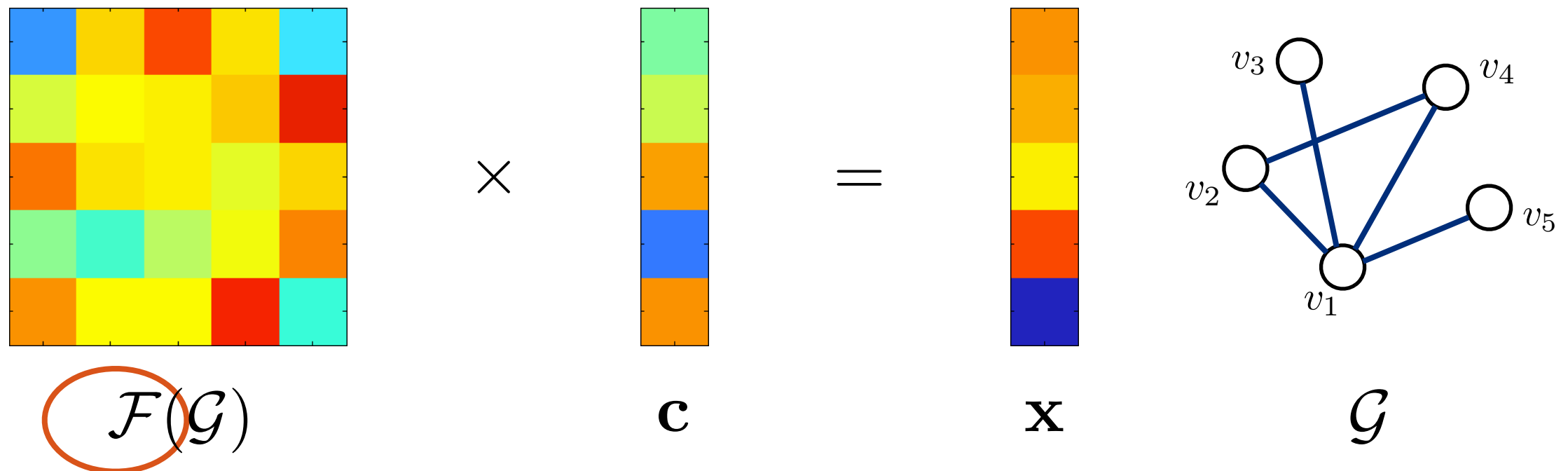
\mathbf{x}



\mathcal{G}

GSP for graph learning

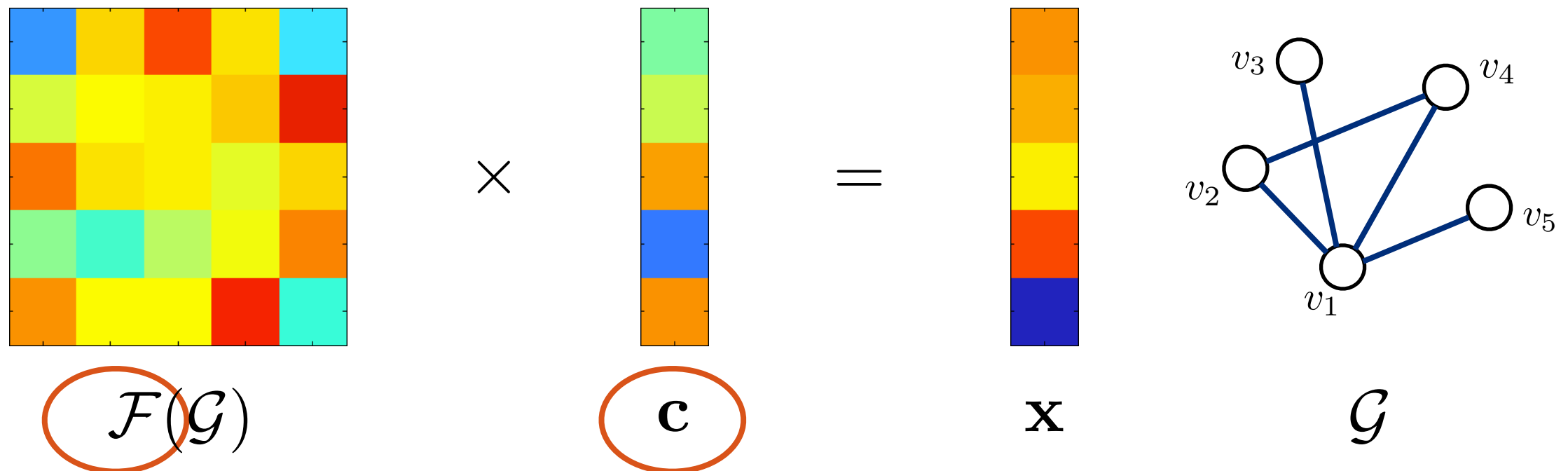
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- assumption on \mathbf{c} also determines signal characteristics

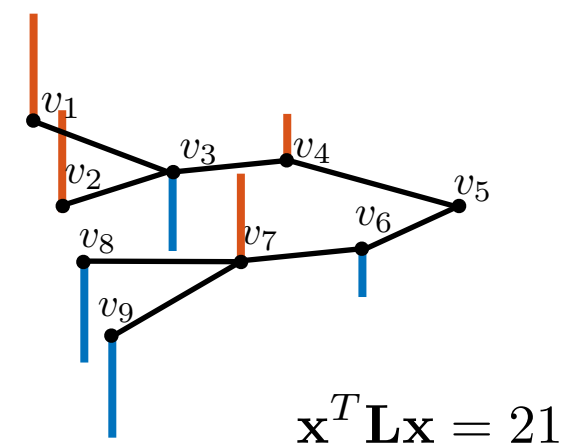
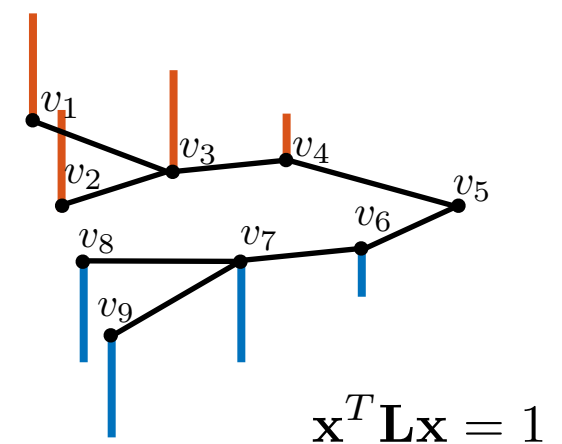
Model 1: Global smoothness

- Signal varies smoothly between all pairs of nodes that are connected
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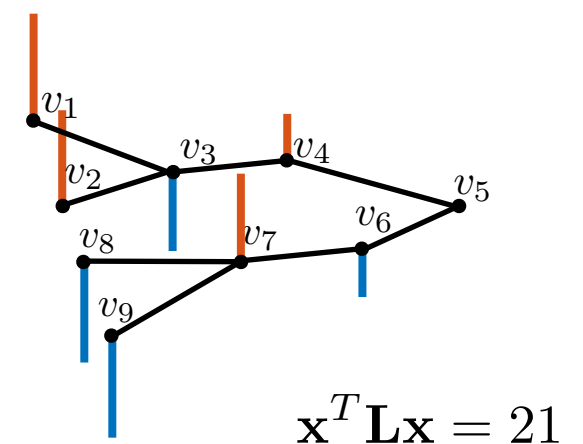
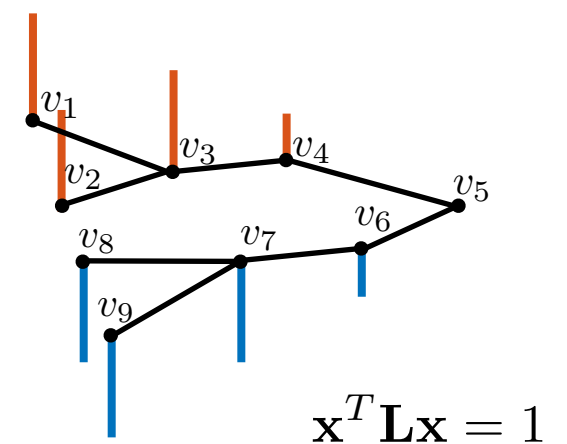
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similar to previous approaches:

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

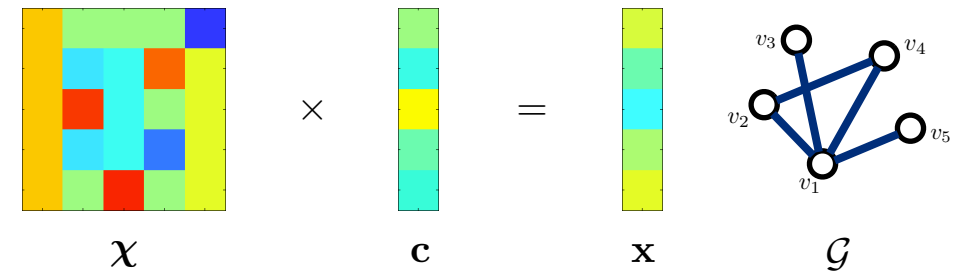
Hu (2013): $\min_{\mathbf{L}} \text{tr}(\mathbf{X}^T \mathbf{L}^s \mathbf{X}) - \beta \|\mathbf{W}\|_F$



Model 1: Global smoothness

- Dong et al. (2016)

- $\mathcal{F}(\mathcal{G}) = \chi$ (eigenvector matrix of \mathbf{L})
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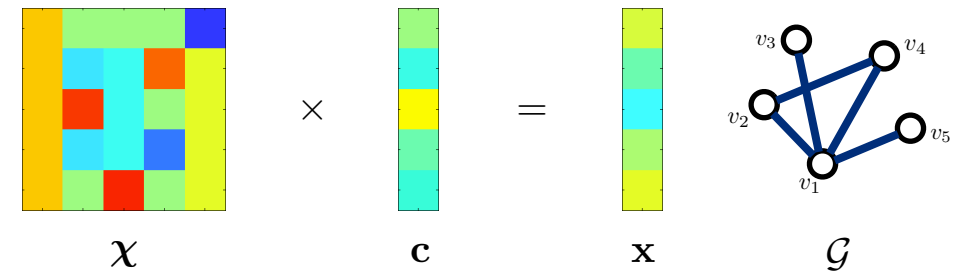


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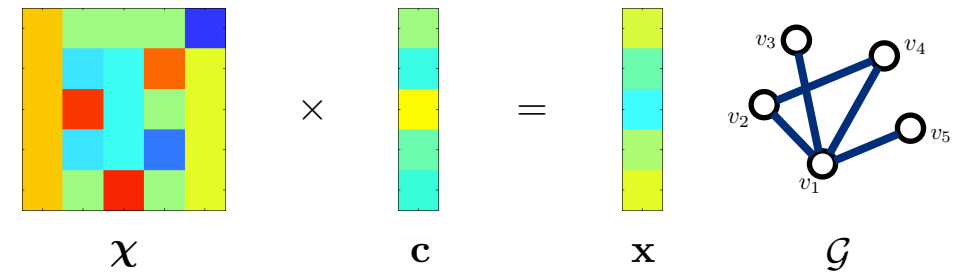
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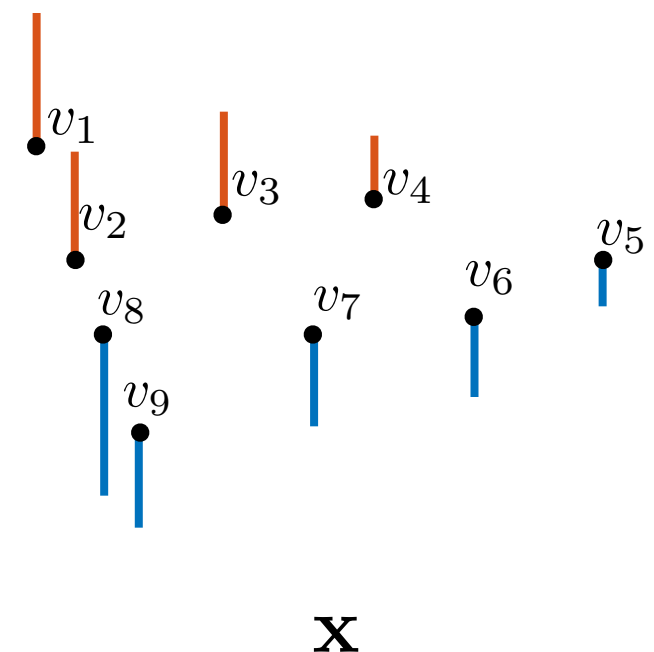
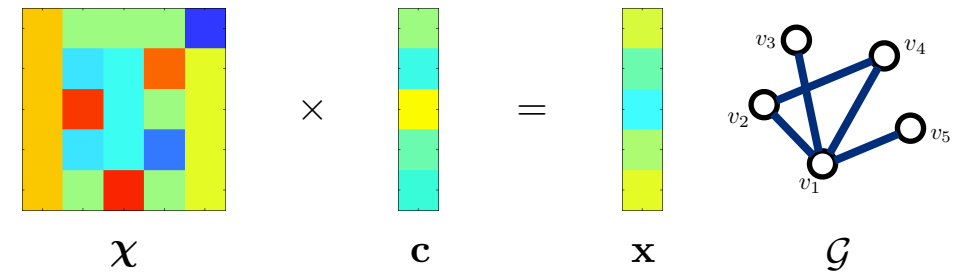
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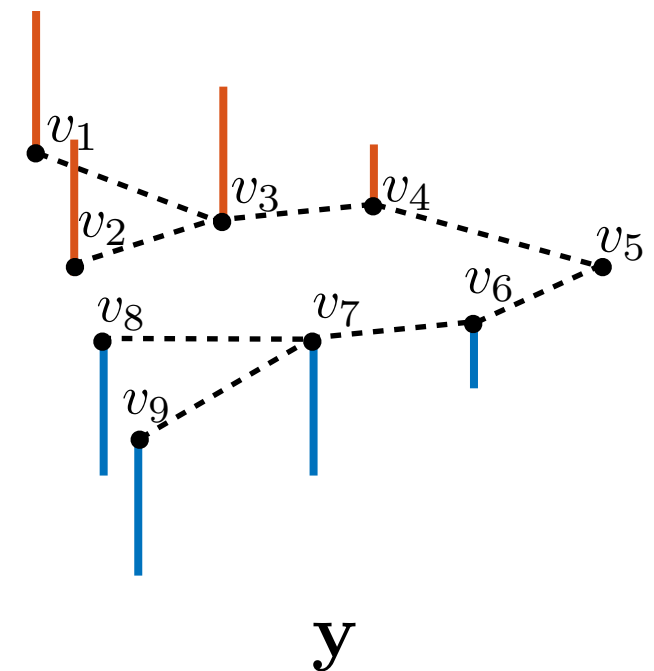
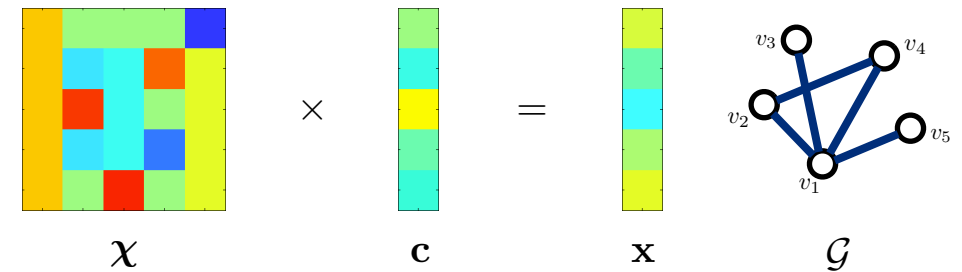
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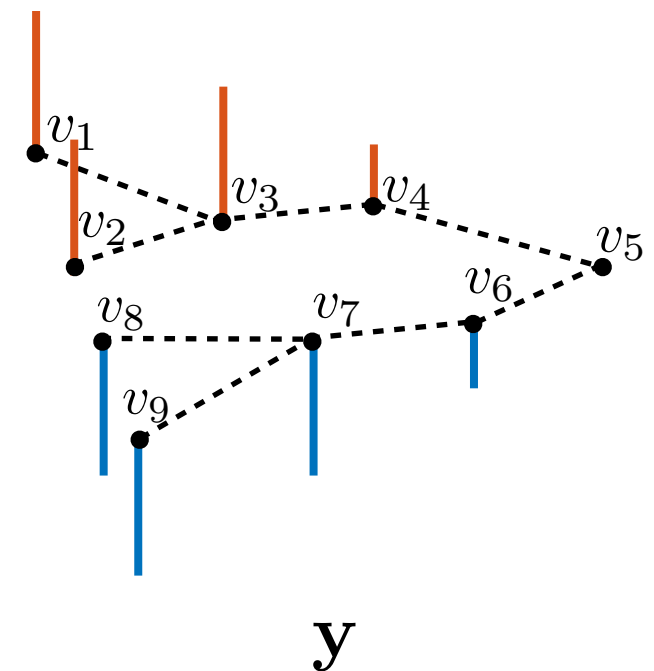
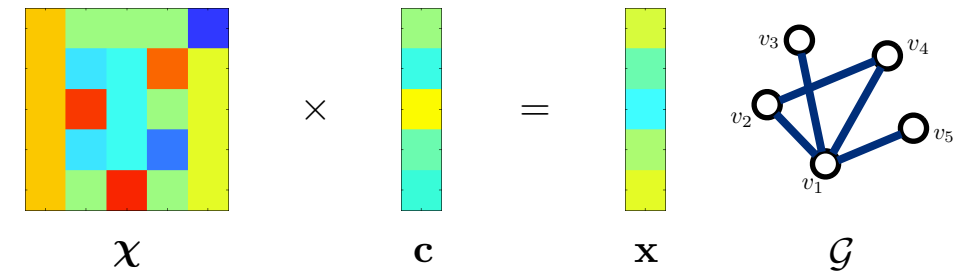
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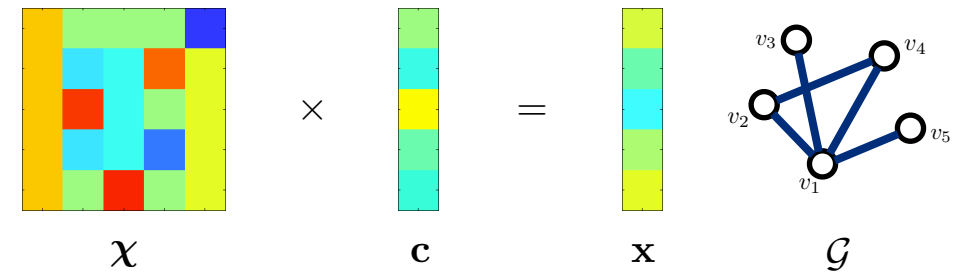
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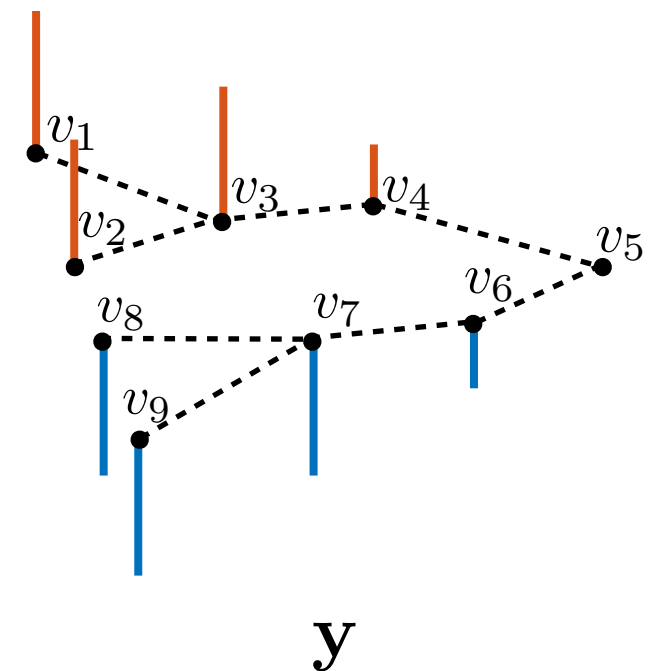
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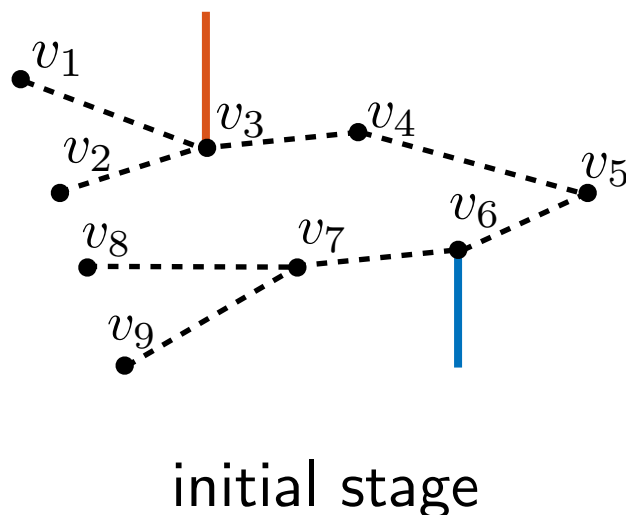
learning enforces signal property (global smoothness)

Model 2: Spectral filtering

- Signals are outcome of applying filtering to latent (input) signals
- Filtering often corresponds to a diffusion process on graphs (different spectral characteristics or localisation properties)
- Example: movement of people/vehicles in transportation network

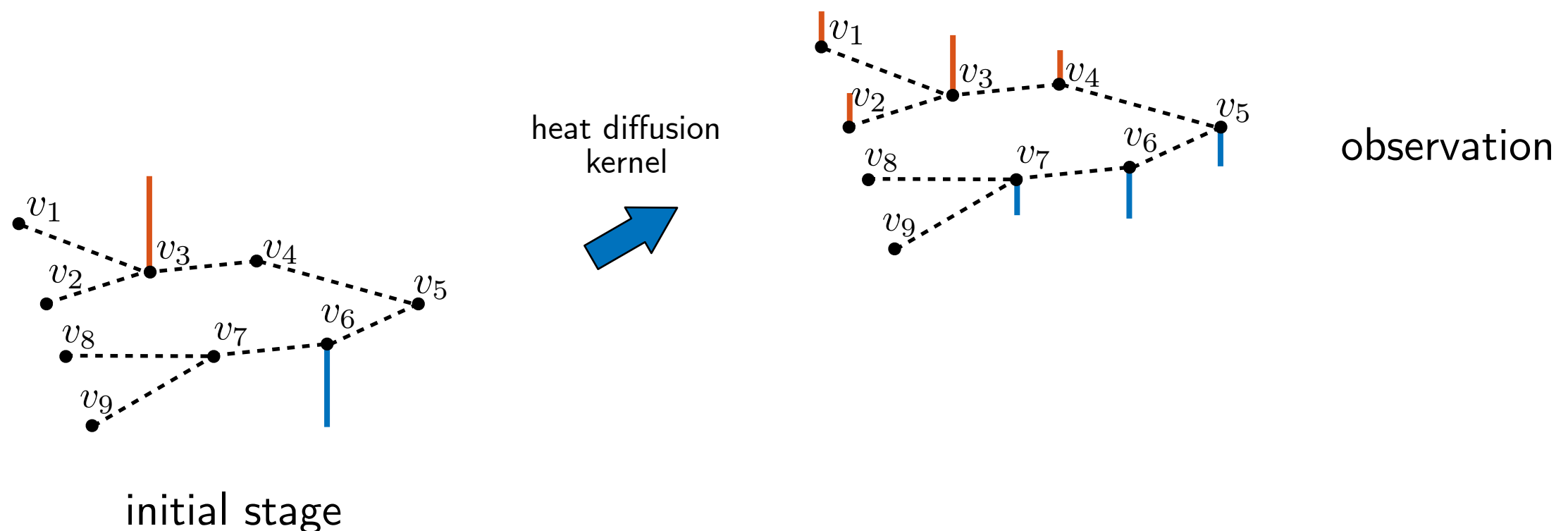
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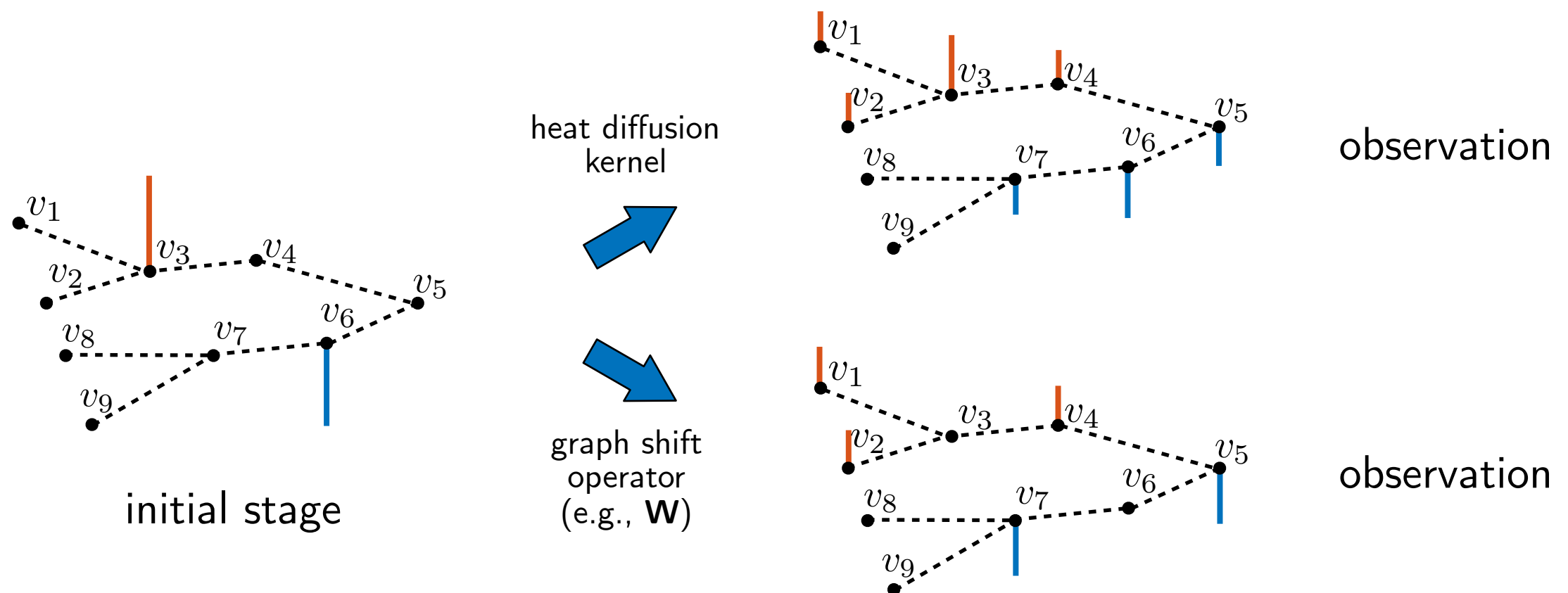
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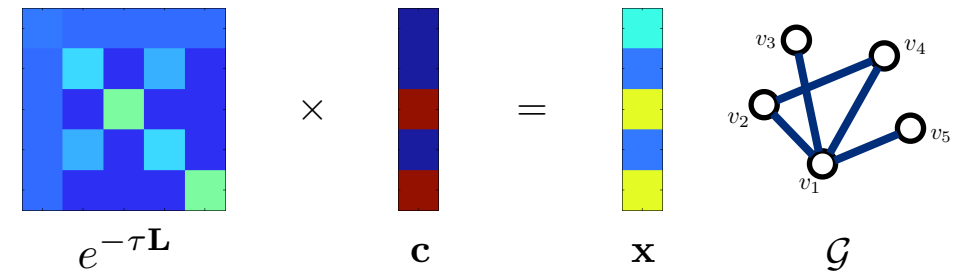
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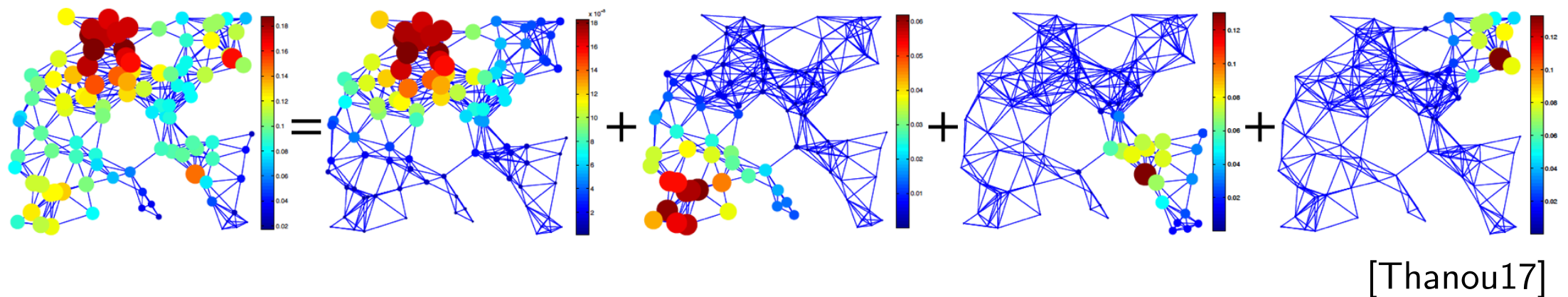
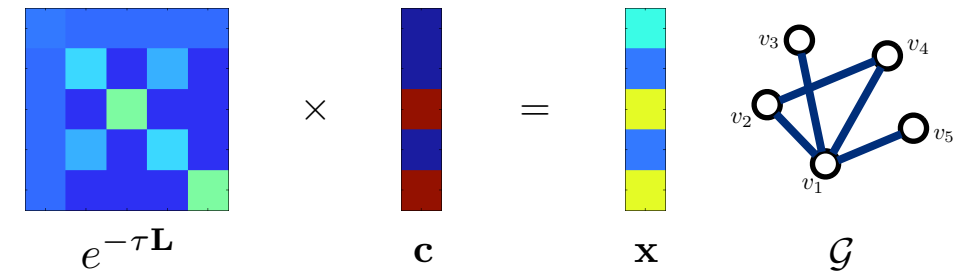
- Thanou et al. (2017)
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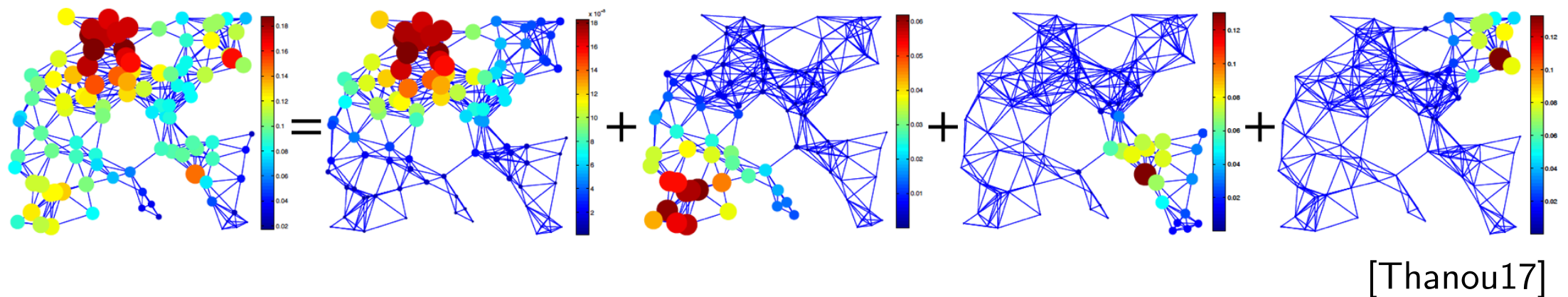
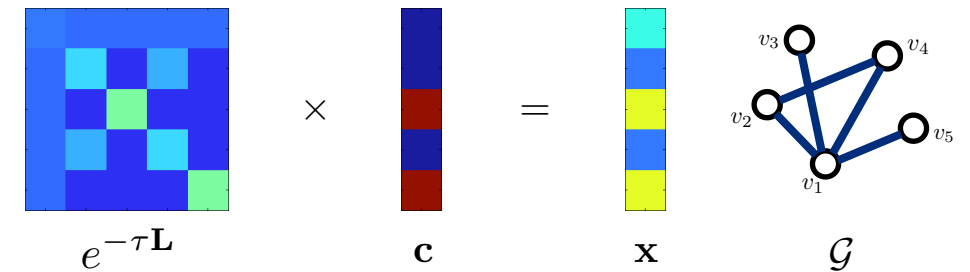
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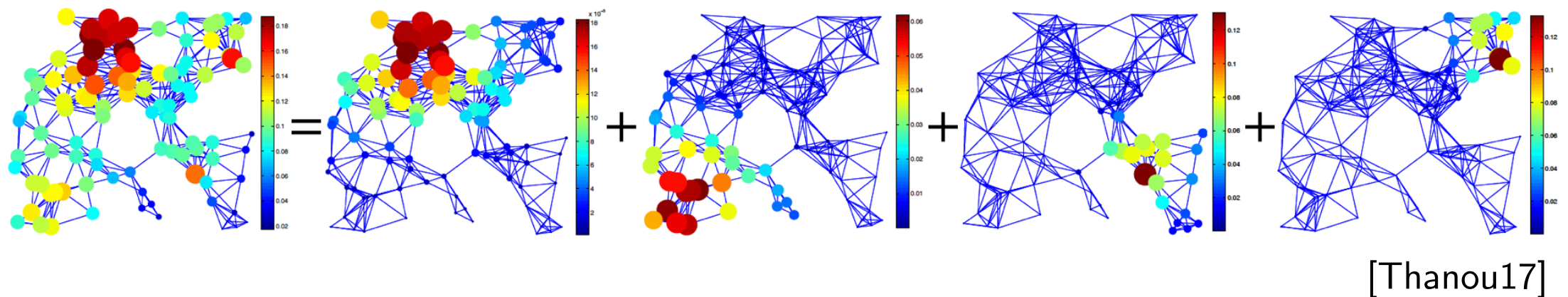
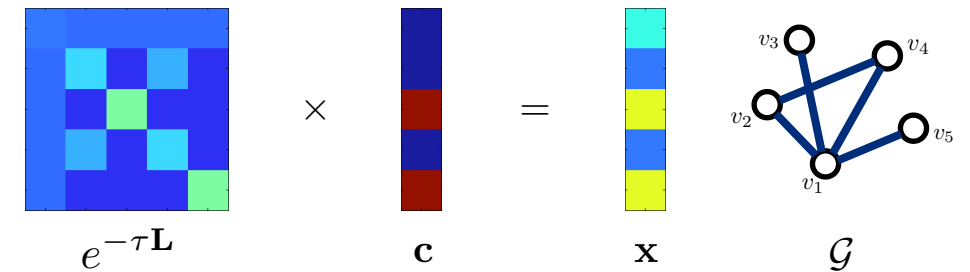


$$\min_{\mathbf{L}, \mathbf{C}, \tau} \|\mathbf{X} - \mathcal{F}\mathbf{C}\|_F^2 + \alpha \sum_{m=1}^M \|\mathbf{c}_m\|_1 + \beta \|\mathbf{L}\|_F^2 \quad \text{s.t.} \quad \mathcal{F} = [e^{-\tau_1 \mathbf{L}}, e^{-\tau_2 \mathbf{L}}, \dots, e^{-\tau_S \mathbf{L}}]$$

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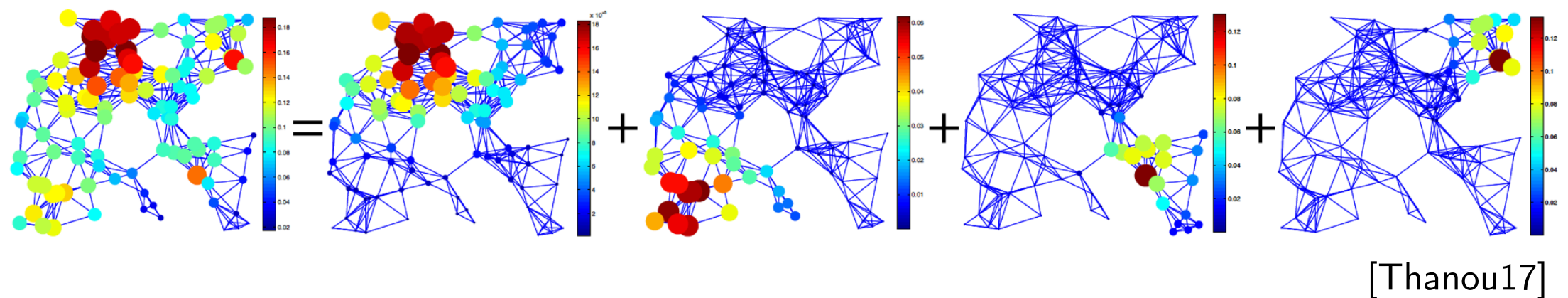
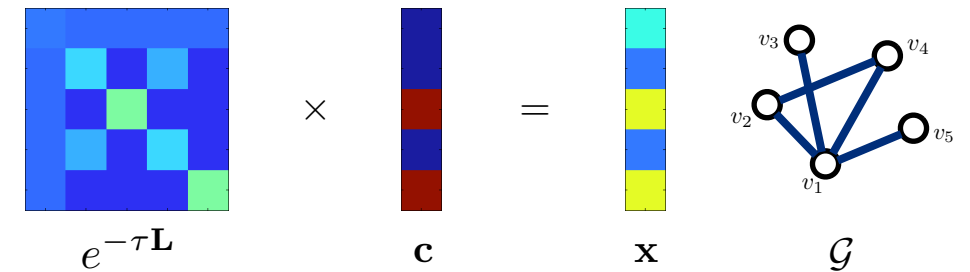


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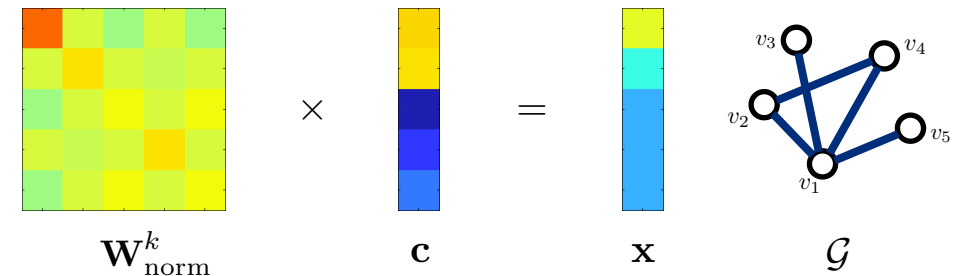
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local (instead of global) signal characteristics
can be extended to general polynomial case

Model 2: Spectral filtering

- Pasdeloup et al. (2017)

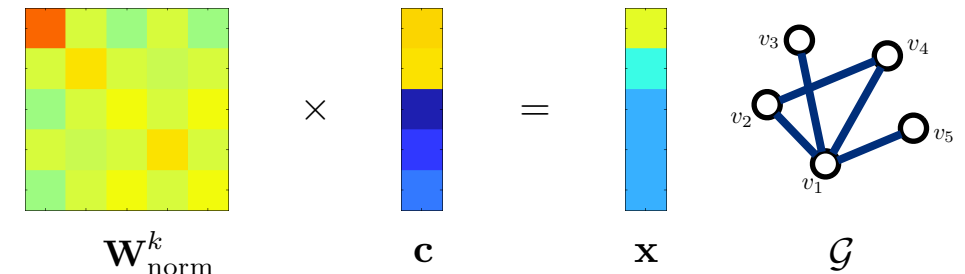
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- Gaussian assumption on \mathbf{c} : $\mathbf{c} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
- two-step approach:
 - estimate eigenvector matrix of graph operator from sample covariance:



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

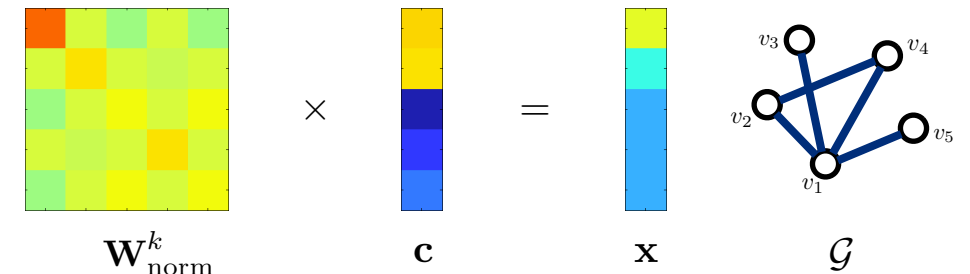
Model 2: Spectral filtering

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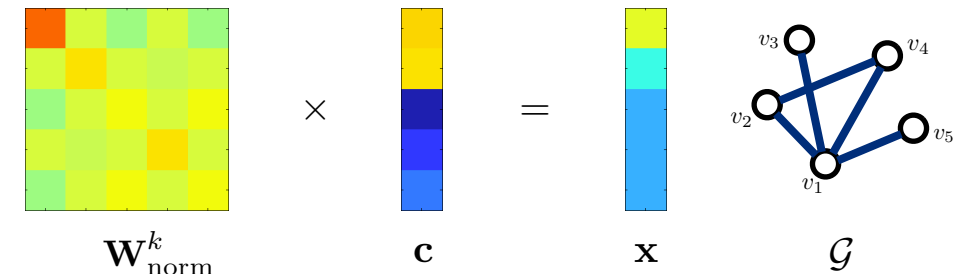
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diffusion process based on different operator

statistical vs structural (Thanou et al.) assumption on \mathbf{c}

“graph-centric”: cost on graph operators instead of signals

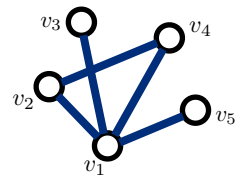
Model 3: Causal dependency on graphs

- Signals are causal outcome of current or past observations (spectral characteristics depending on dependence structure)
- Example: evolution of individual behaviour due to influence of different friends at different timestamps
- Characterised by vector autoregressive models (VARMs) or structural equation models (SEMs)
 - VARMs exploits relation between present and past
 - SEMs exploits relation between vertices at present

Model 3: Causal dependency on graphs

- Mei and Moura (2017)

- $\mathcal{F}_s(\mathcal{G}) = \mathbf{P}_s(\mathbf{W})$: polynomial of \mathbf{W} of degree s
- define \mathbf{c}_s as $\mathbf{x}[t-s]$

$$\sum_{s=1}^S \left(\begin{array}{c} \text{Heatmap} \\ \mathbf{P}_s(\mathbf{W}) \end{array} \times \begin{array}{c} \text{Vector} \\ \mathbf{x}[t-s] \end{array} \right) = \begin{array}{c} \text{Heatmap} \\ \mathbf{x} \end{array} \quad \mathcal{G}$$


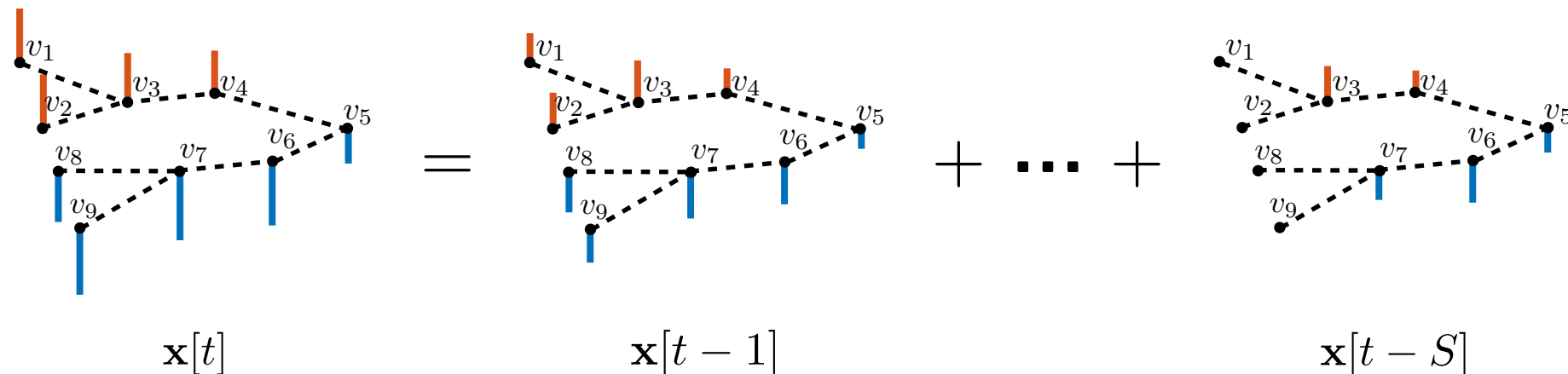
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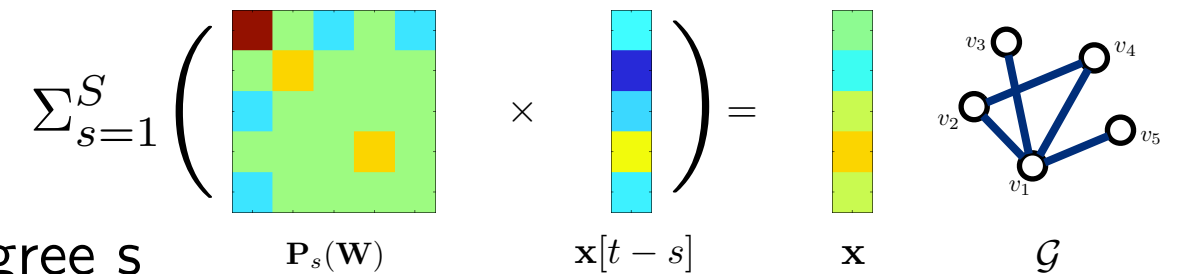
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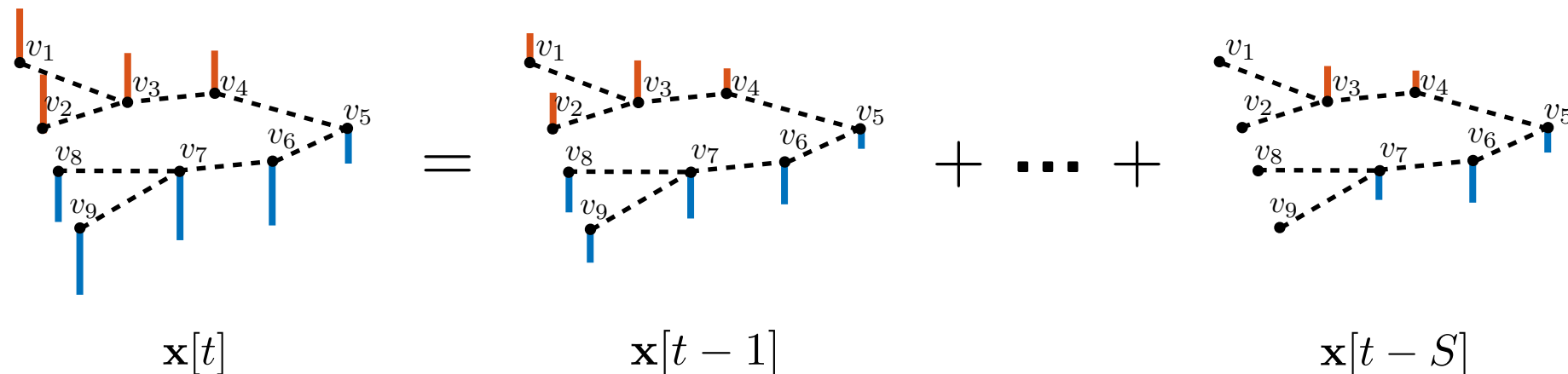


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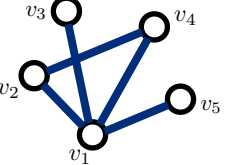


$$\min_{\mathbf{W}, \mathbf{a}} \frac{1}{2} \sum_{k=S+1}^K \|\mathbf{x}[k] - \sum_{s=1}^S \mathbf{P}_s(\mathbf{W}) \mathbf{x}[k-s]\|_2^2 + \lambda_1 \|\text{vec}(\mathbf{W})\|_1 + \lambda_2 \|\mathbf{a}\|_1$$

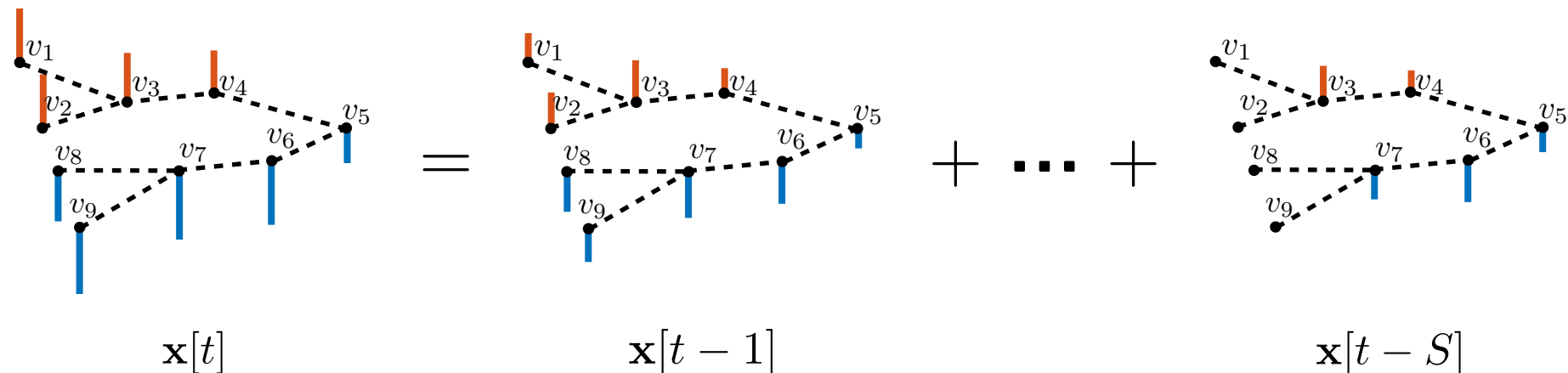
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\mathcal{G}



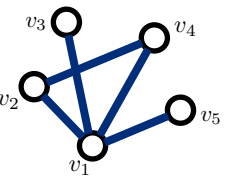
$$\min_{\mathbf{W}, \mathbf{a}} \frac{1}{2} \sum_{k=S+1}^K \left(\left\| \mathbf{x}[k] - \sum_{s=1}^S \mathbf{P}_s(\mathbf{W}) \mathbf{x}[k-s] \right\|_2^2 + \lambda_1 \left\| \text{vec}(\mathbf{W}) \right\|_1 + \lambda_2 \left\| \mathbf{a} \right\|_1 \right)$$

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

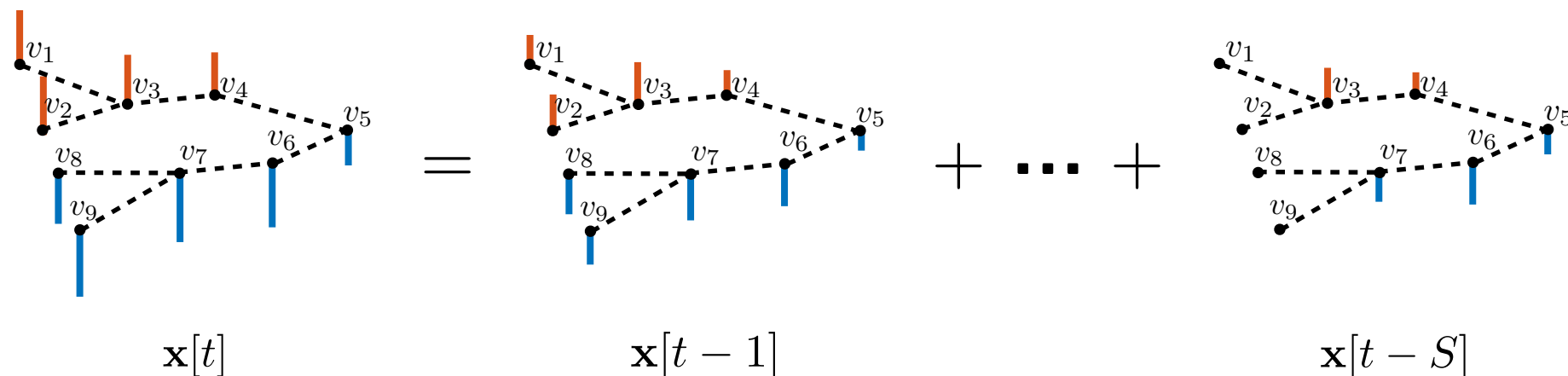
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$\mathbf{P}_s(\mathbf{W})$ $\mathbf{x}[t-s]$ \mathbf{x} \mathcal{G}



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

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

good for inferring causal relations between signals
can be combined with SEMs and kernelised

Comparison of different GSP methods

Table 1. Comparisons between different GSP-based approaches to graph learning.

Method	Signal Model	Assumption		Learning Output	Edge Directionality
		$\mathcal{F}(\mathcal{G})$	\mathbf{c}		
Dong et al. [39]	Global smoothness	Eigenvector matrix	i.i.d. Gaussian	Laplacian	Undirected
Kalofolias et al. [40]	Global smoothness	Eigenvector matrix	i.i.d. Gaussian	Adjacency matrix	Undirected
Egilmez et al. [41]	Global smoothness	Eigenvector matrix	i.i.d. Gaussian	Generalized Laplacian	Undirected
Chepuri et al. [42]	Global smoothness	Eigenvector matrix	i.i.d. Gaussian	Adjacency matrix	Undirected
Pasdeloup et al. [46]	Spectral filtering (diffusion by adjacency)	Normalized adjacency matrix	i.i.d. Gaussian	Normalized adjacency matrix normalized Laplacian	Undirected
Segarra et al. [45]	Spectral filtering (diffusion by graph shift operator)	Graph shift operator	i.i.d. Gaussian	Graph shift operator	Undirected
Thanou et al. [47]	Spectral filtering (heat diffusion)	Heat kernel	Sparsity	Laplacian	Undirected
Mei and Moura [55]	Causal dependency (SVAR)	Polynomials of adjacency matrix	Past signals	Adjacency matrix	Directed
Baingana et al. [62]	Causal dependency (SEM)	Adjacency matrix	Present signal	Time-varying adjacency matrix	Directed
Shen et al. [54]	Causal dependency (SVARM)	Polynomials of adjacency matrix	Past and present signals	Adjacency matrix	Directed

[Dong19]

Connection with broad literature

- Global smoothness of graph signals is also promoted in Graphical Lasso

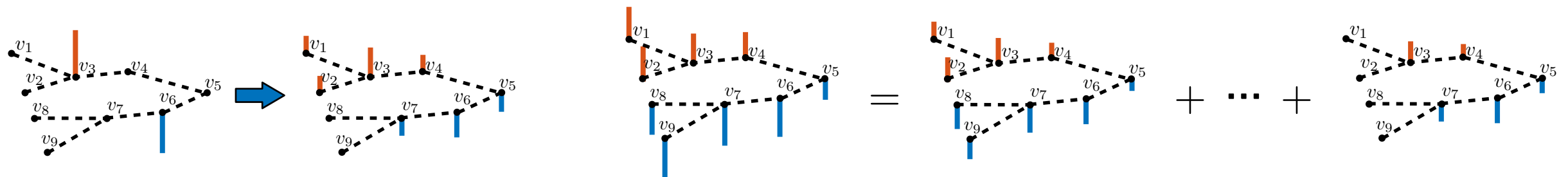
Lake (2010):
$$\max_{\Theta = \mathbf{L} + \frac{1}{\sigma^2} \mathbf{I}} \log \det \Theta - \frac{1}{M} \text{tr}(\mathbf{X} \mathbf{X}^T \Theta) - \rho \|\Theta\|_1$$

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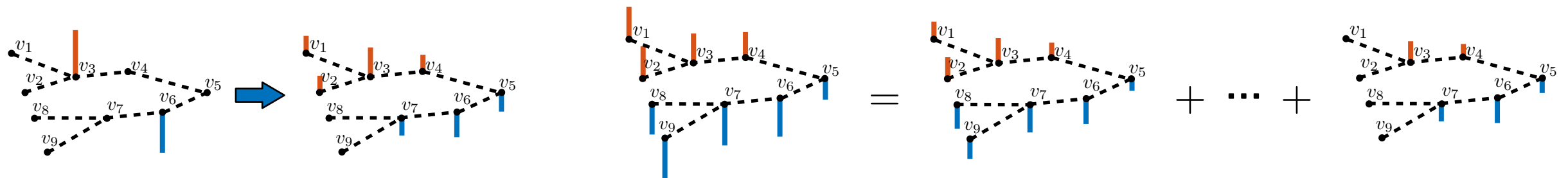


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- Models based on spectral filtering or causal dependency lead to generative process of signals, similarly to traditional physically motivated models



- GSP approaches offer design flexibility (via \mathbf{F} and \mathbf{c}) and extend beyond a Gaussian statistical model or a simple diffusion model

Applications

- Image coding and compression (review of [Chung18])
 - images are natural graph signals on regular grid
 - learning adaptive edge weights for structure-aware transform coding
 - more efficient image compression

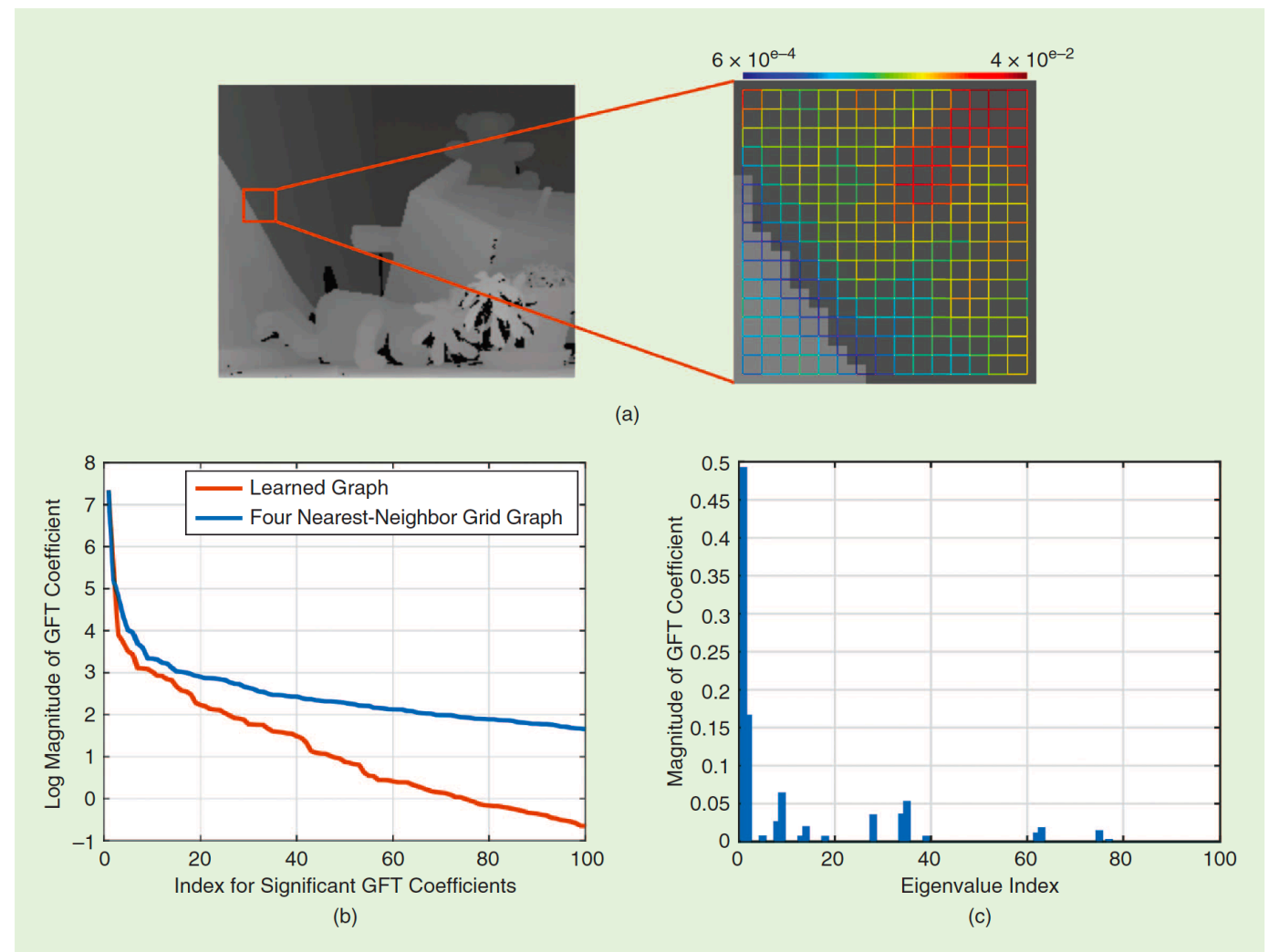
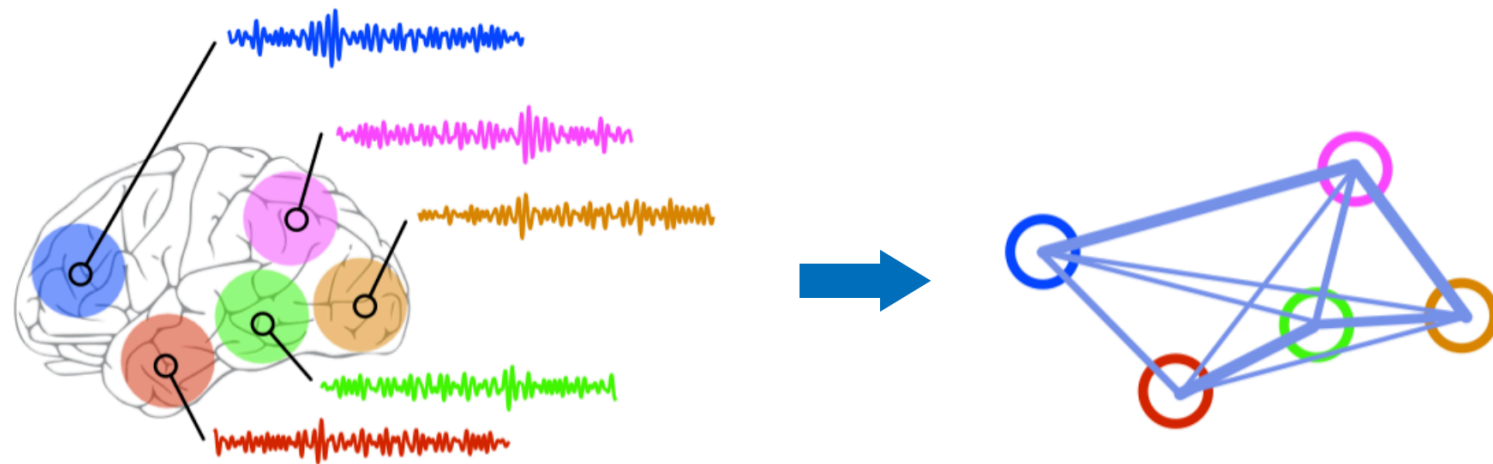


FIGURE 10. Inferring a graph for image coding. (a) The graph learned on a random patch of the image Teddy using [69]. (b) A comparison between the GFT coefficients of the image signal on the learned graph and the four nearest-neighbor grid graph. The coefficients are ordered decreasingly by log magnitude. (c) The GFT coefficients of the graph weights.

[Fracastoro17]

Applications

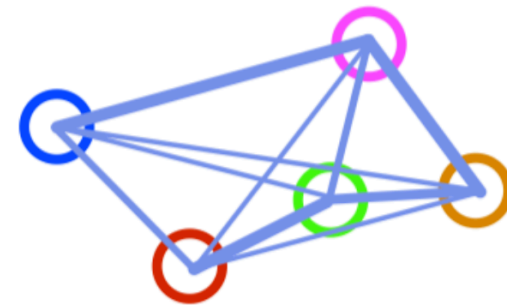
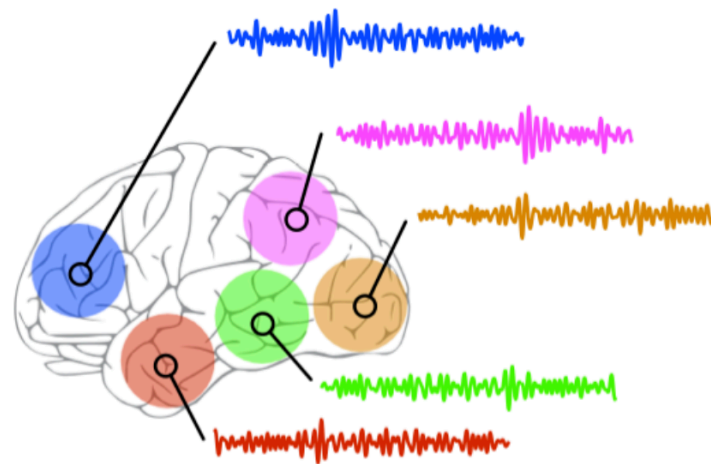
- Brain signal analysis (review of [Huang18])
 - learning functional connectivity of brain regions



[Richiardi13]

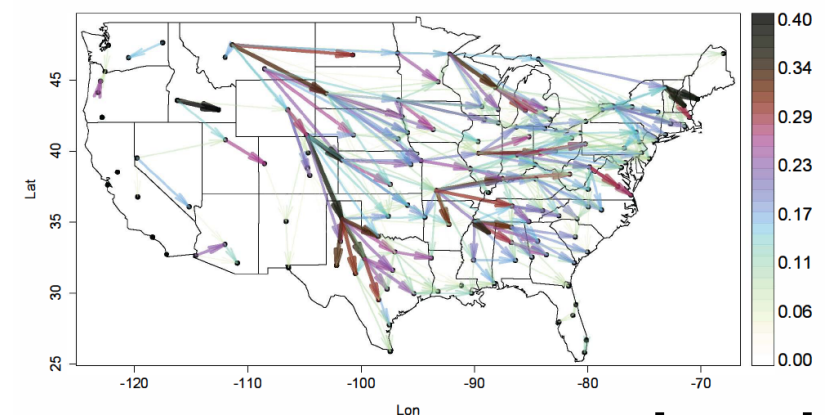
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[Richiardi13]

- Other application domains
 - learning meteorology graph using temperatures
 - learning commuting graph using traffic volume
 - learning political relations using voting data

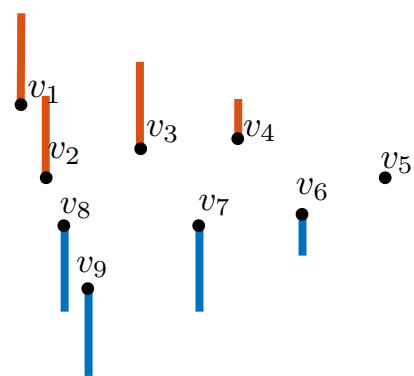


[Mei17]

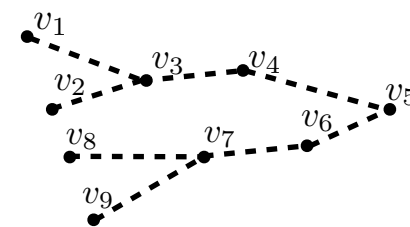
Outline

- A (very partial) literature overview
- A signal processing perspective
 - A brief introduction to graph signal processing (GSP)
 - GSP approaches for graph learning
- Concluding remarks

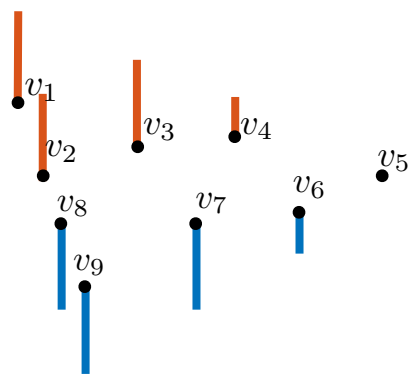
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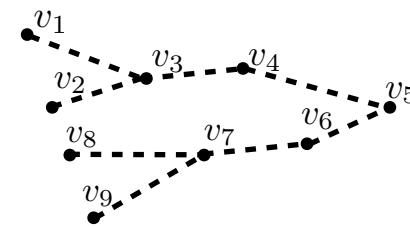
GSP for graph learning



Concluding remarks



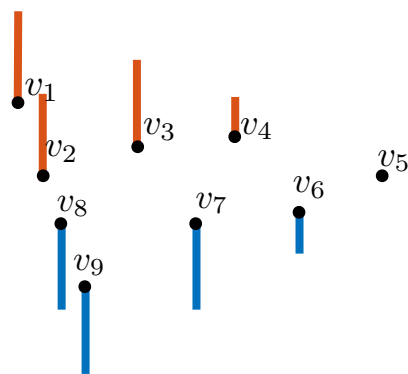
GSP for graph learning



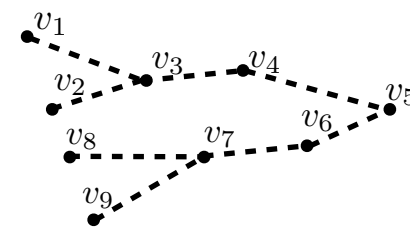
input signals

- partial observations
- sequential observations

Concluding remarks



GSP for graph learning



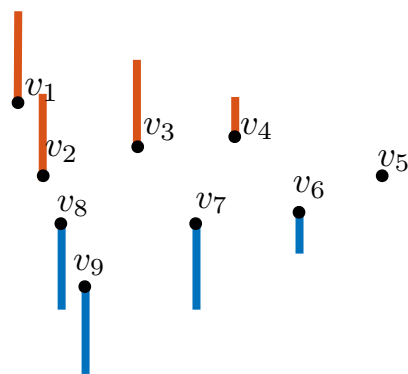
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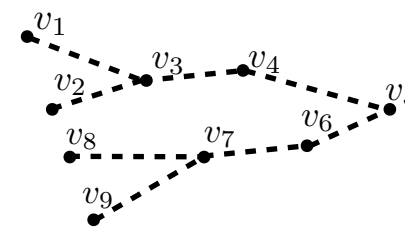
learning outcome

- directed graphs
- time-varying (dynamic) graphs
- graphs with certain properties
- intermediate graph representation
- uncertainty in learned structure

Concluding remarks



GSP for graph learning



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- sequential observations

signal/graph model

- beyond smoothness: localisation in vertex-frequency domain
- adapt to specific input/output

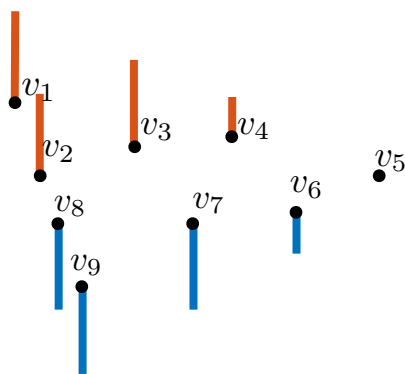
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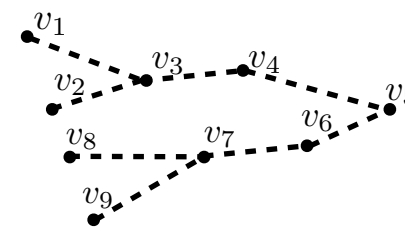
Concluding remarks

theoretical consideration

- performance guarantee
- computational efficiency



GSP for graph learning



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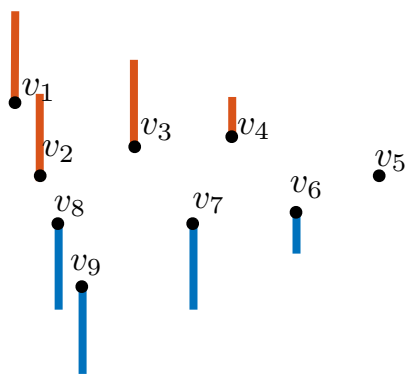
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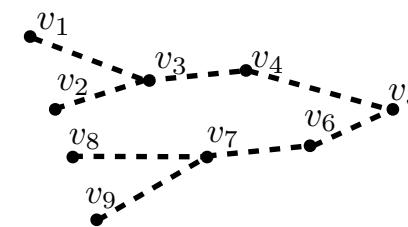
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objective of graph learning

- for traditional graph-based learning, e.g., clustering, dim. reduction, ranking
- integrate inference with subsequent data analysis (targeted applications)



GSP for graph learning



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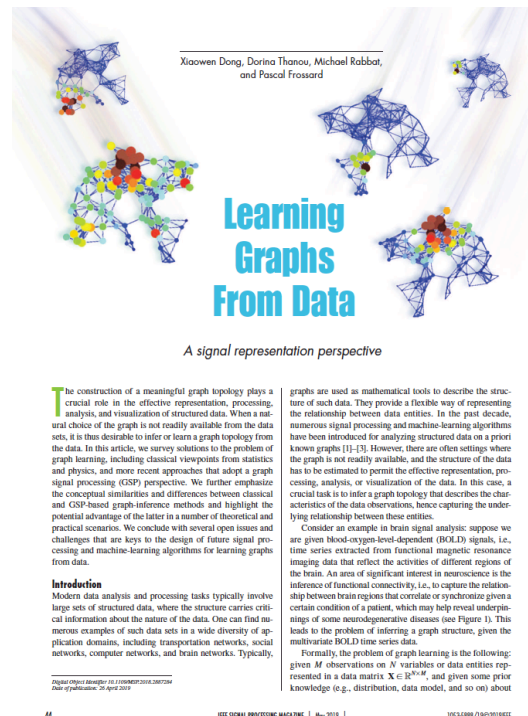
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Papers & Resources & Acknowledgement



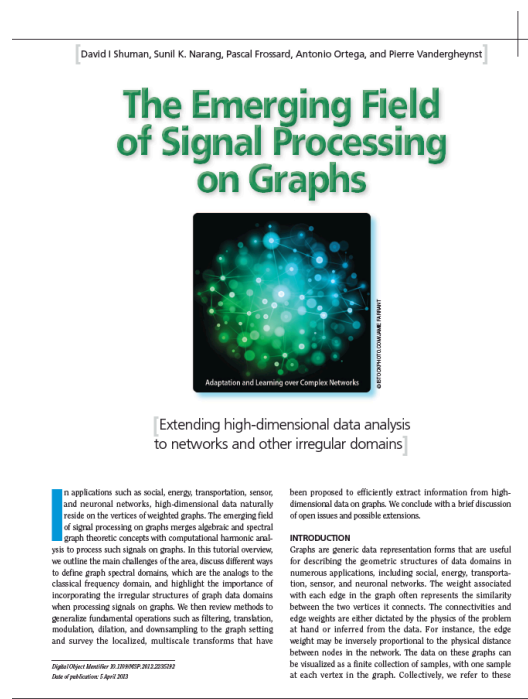
Dorina Thanou



Mike Rabbat



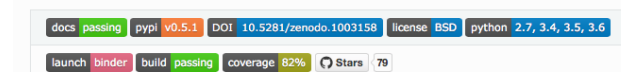
Pascal Frossard



The **Graph Signal Processing toolbox** is an easy to use matlab toolbox that performs a wide variety of operations on graphs, from simple ones like filtering to advanced ones like interpolation or graph learning. You can create all sorts of filterbanks including wavelets and Gabor. It is based on spectral graph theory and many of the features can scale to very large graphs.

<https://epfl-lts2.github.io/gspbox-html/>

PyGSP: Graph Signal Processing in Python



The PyGSP is a Python package to ease [Signal Processing on Graphs](#). It is a free software, distributed under the BSD license, and available on [PyPI](#). The documentation is available on [Read the Docs](#) and development takes place on [GitHub](#). (A [Matlab counterpart](#) exists.)

<https://pygsp.readthedocs.io/en/stable/>

More: <http://web.media.mit.edu/~xdong/resource.html>

Thank you!