# Graph signal processing

Concepts, tools and applications in neuroscience

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NISOx, Big Data Institute, February 2019





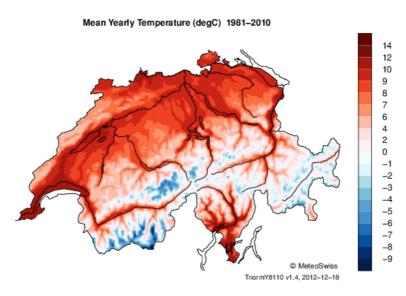
#### Outline

- Motivation
- Graph signal processing (GSP): Basic concepts
- Spectral filtering: Basic tools of GSP
- Connection with literature
- Applications in neuroscience

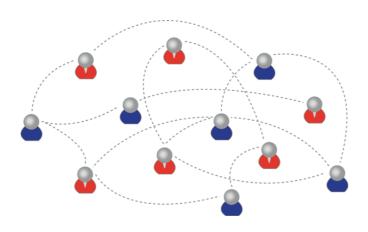
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#### Data are often structured



Temperature data



Social network data

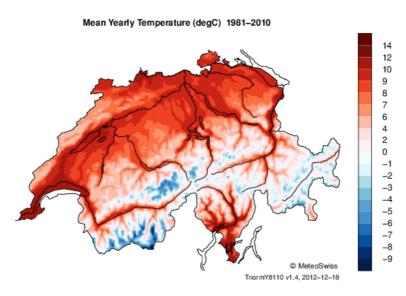


Traffic data

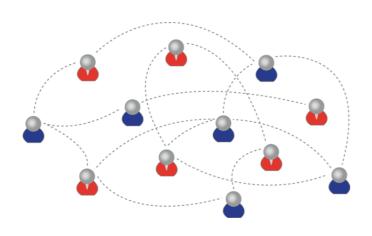


Neuroimaging data

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Temperature data



Social network data



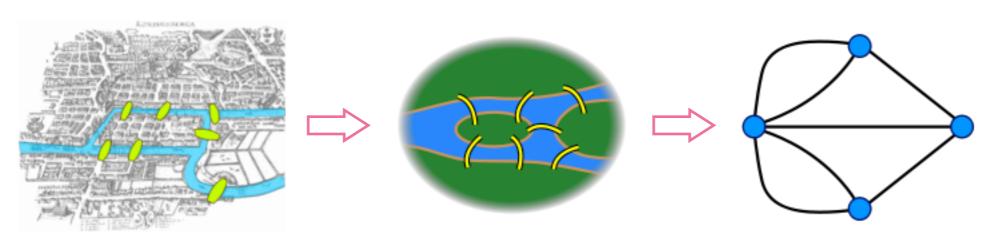
Traffic data



**Neuroimaging data** 

We need to take into account the structure behind the data

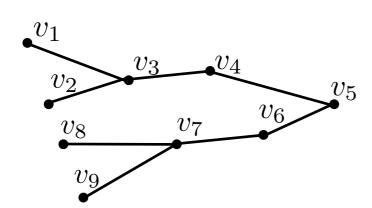
• Efficient representations for pairwise relations between entities



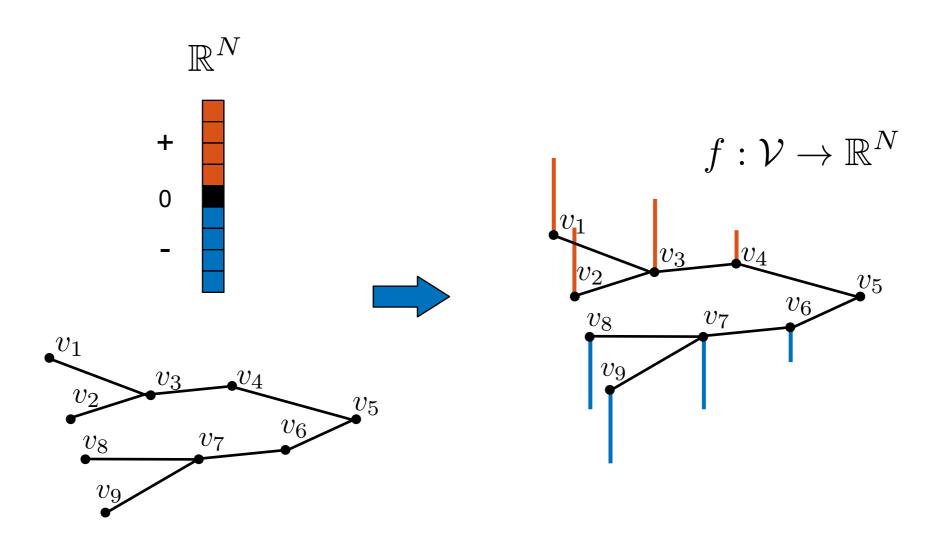
The Königsberg Bridge Problem [Leonhard Euler, 1736]



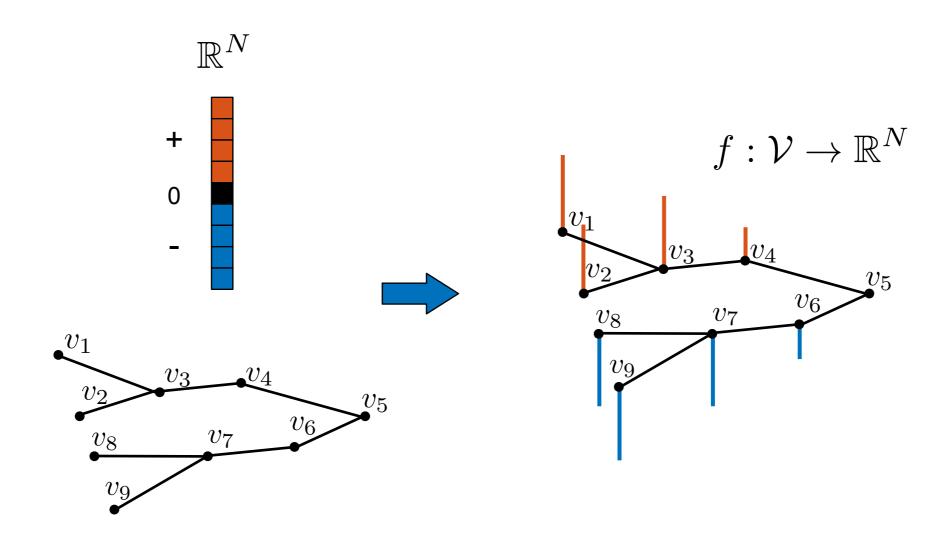
• Efficient representations for pairwise relations between entities



- Efficient representations for pairwise relations between entities
- Structured data can be represented by graph signals

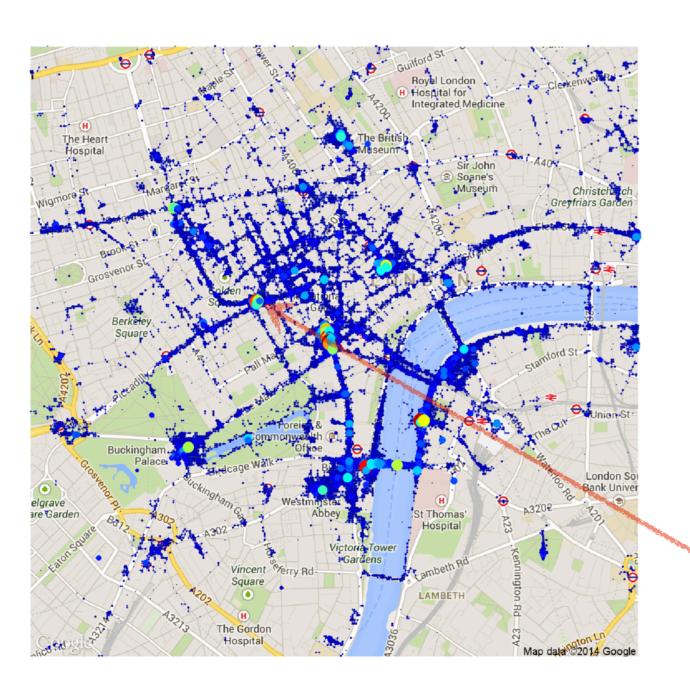


- Efficient representations for pairwise relations between entities
- Structured data can be represented by graph signals

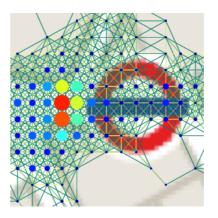


Takes into account both structure (edges) and data (values at vertices)

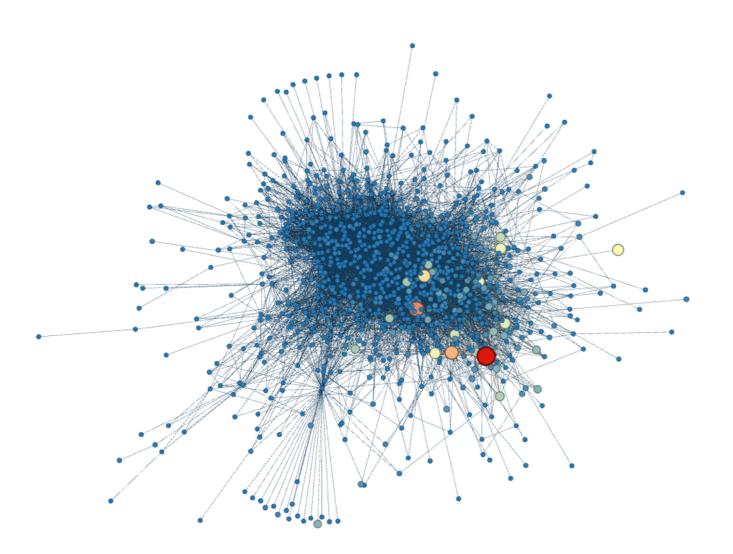
#### Graph signals are pervasive



- 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

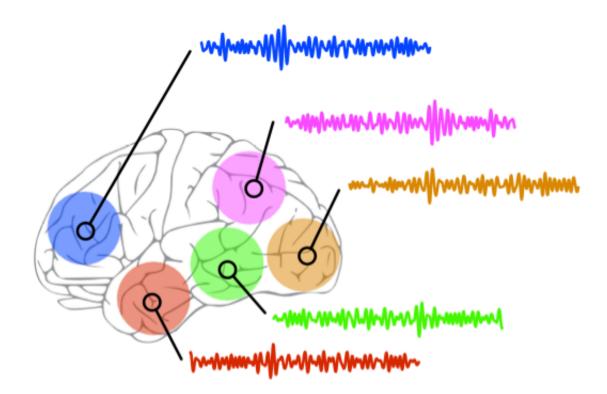


## Graph signals are pervasive



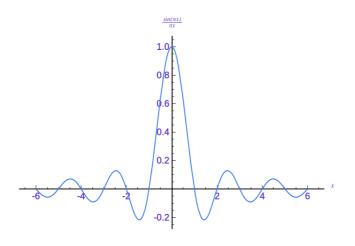
- Vertices:
  - 1000 Twitter users
- Edges:
  - following relationship among users
- Signal:
  - # Apple-related hashtags they have posted in six weeks

#### Graph signals are pervasive

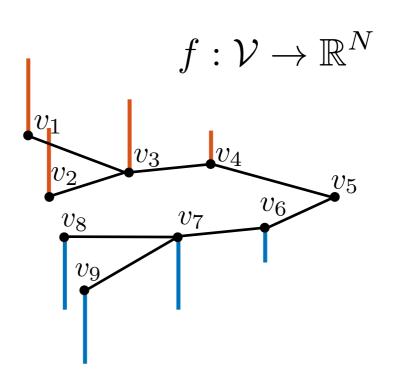


- Vertices:
  - brain regions
- Edges:
  - structural connectivity between brain regions
- Signal:
  - blood-oxygen-level-dependent
     (BOLD) time series

#### Research challenges



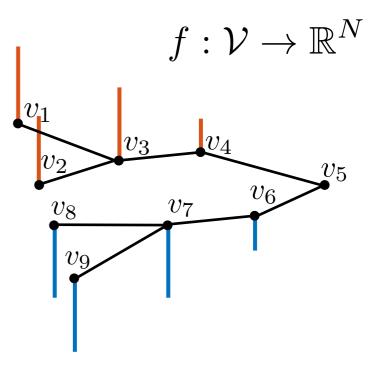




How to generalise classical signal processing tools on irregular domains such as graphs?

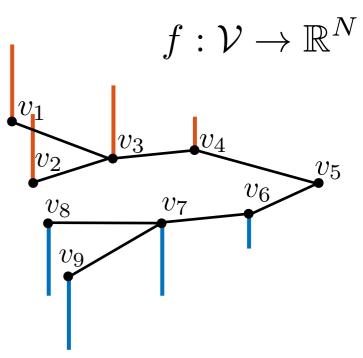
## Graph signal processing

- Graph signals provide a nice compact format to encode structure within data
- Generalisation of classical signal processing tools can greatly benefit analysis of such data
- Numerous applications: Transportation, biomedical, social network analysis, etc.



#### Graph signal processing

- Graph signals provide a nice compact format to encode structure within data
- Generalisation of classical signal processing tools can greatly benefit analysis of such data
- Numerous applications: Transportation, biomedical, social network analysis, etc.
- An increasingly rich literature
  - classical signal processing
  - algebraic and spectral graph theory
  - computational harmonic analysis
  - machine learning

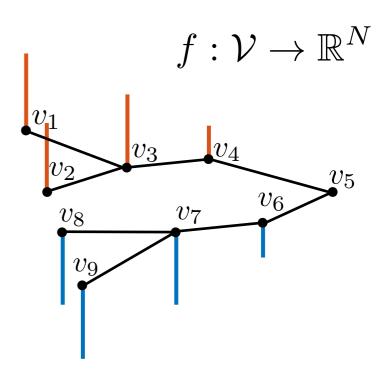


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## Two paradigms

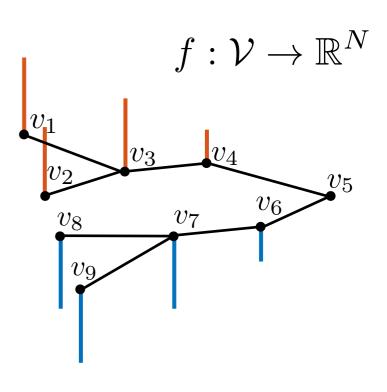
- The main approaches can be categorised into two families:
  - vertex (spatial) domain designs
  - frequency (graph spectral) domain designs



#### Two paradigms

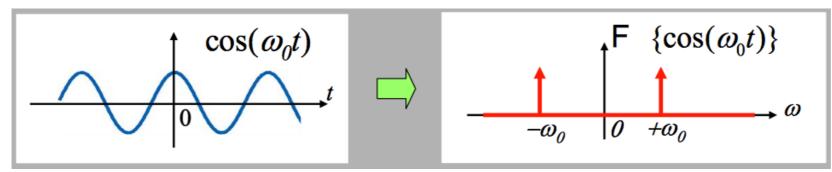
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Important for analysis of signal properties

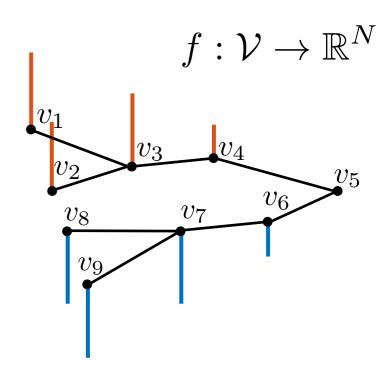


#### Need for frequency

 Classical Fourier transform provides the frequency domain representation of the signals

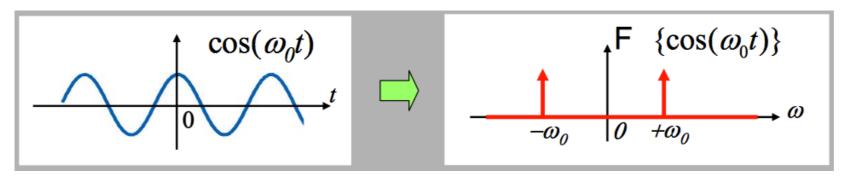


Source: <a href="http://www.physik.uni-kl.de">http://www.physik.uni-kl.de</a>



#### Need for frequency

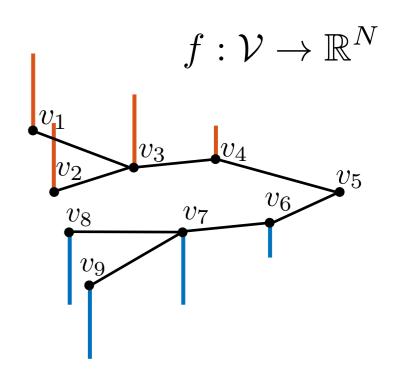
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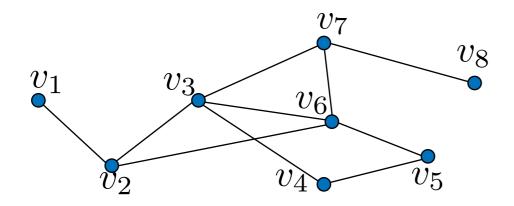


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A notion of frequency for graph signals:

We need the graph Laplacian matrix



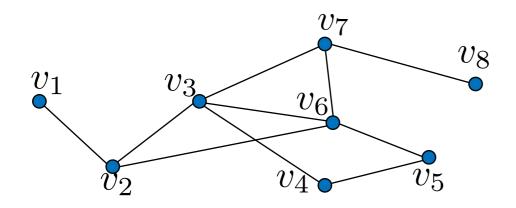


Weighted and undirected graph:

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

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

W

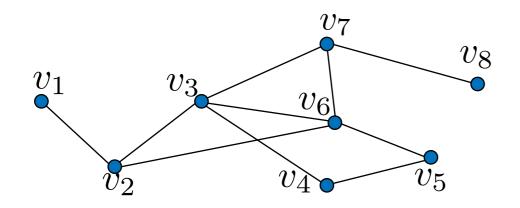


Weighted and undirected graph:

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

$$D = \operatorname{diag}(d(v_1), \cdots, d(v_N))$$

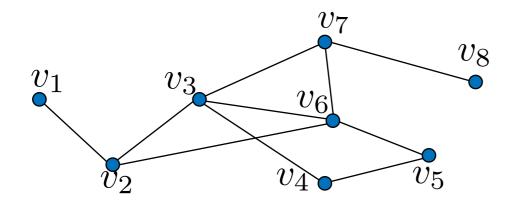
$$egin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} egin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \ 1 & 0 &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



Weighted and undirected graph:

$$\mathcal{G}=\{\mathcal{V},\mathcal{E}\}$$
 
$$D=\mathrm{diag}(d(v_1),\cdots,d(v_N))$$
 
$$L=D-W \qquad ext{Equivalent to G!}$$

- Symmetric
- Off-diagonal entries non-positive
- Rows sum up to zero



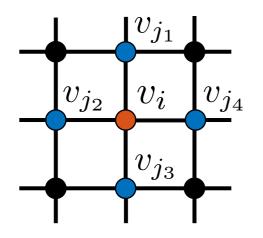
Weighted and undirected graph:

$$\mathcal{G} = \{\mathcal{V}, \mathcal{E}\}$$
 $D = \operatorname{diag}(d(v_1), \cdots, d(v_N))$ 
 $L = D - W$  Equivalent to G!
 $L_{\operatorname{norm}} = D^{-\frac{1}{2}}(D - W)D^{-\frac{1}{2}}$ 

Why graph Laplacian?

#### Why graph Laplacian?

- approximation of the Laplace operator

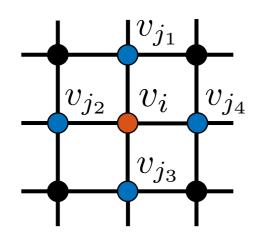


$$(Lf)(i) = 4f(i) - [f(j_1) + f(j_2) + f(j_3) + f(j_4)]$$

standard 5-point stencil for approximating  $-\nabla^2 f$ 

#### Why graph Laplacian?

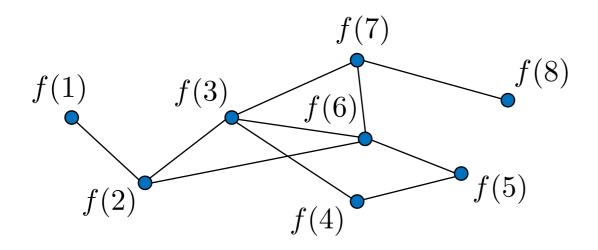
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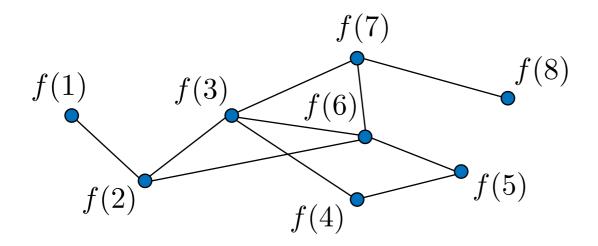
$$(Lf)(i) = 4f(i) - [f(j_1) + f(j_2) + f(j_3) + f(j_4)]$$

standard 5-point stencil for approximating  $-\nabla^2 f$ 

- converges to the Laplace-Beltrami operator (given certain conditions)
- provides a notion of "frequency" on graphs



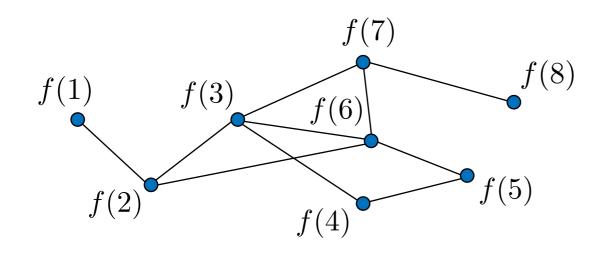
Graph signal  $f:\mathcal{V} 
ightarrow \mathbb{R}^N$ 



Graph signal  $f:\mathcal{V} o\mathbb{R}^N$ 

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

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



Graph signal  $f:\mathcal{V} 
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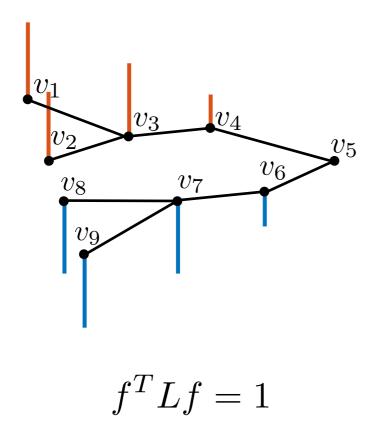
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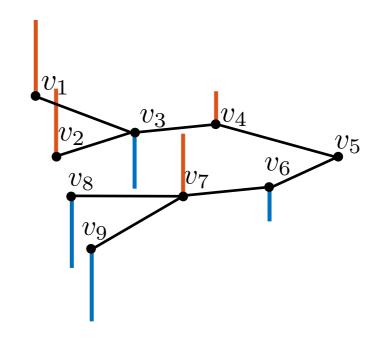
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$$Lf(i) = \sum_{j=1}^{N} W_{ij}(f(i) - f(j))$$

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

A measure of "smoothness"





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

$$L = \begin{bmatrix} 1 & & & 1 \\ \chi_0 & \cdots & \chi_{N-1} \\ \end{bmatrix} \begin{bmatrix} \lambda_0 & & 0 \\ & \ddots & \\ 0 & & \lambda_{N-1} \end{bmatrix} \begin{bmatrix} & & \chi_0 & & \\ & & \ddots & \\ & & & \chi_{N-1} & & \end{bmatrix}$$

$$\chi \qquad \qquad \Lambda \qquad \qquad \chi^T$$

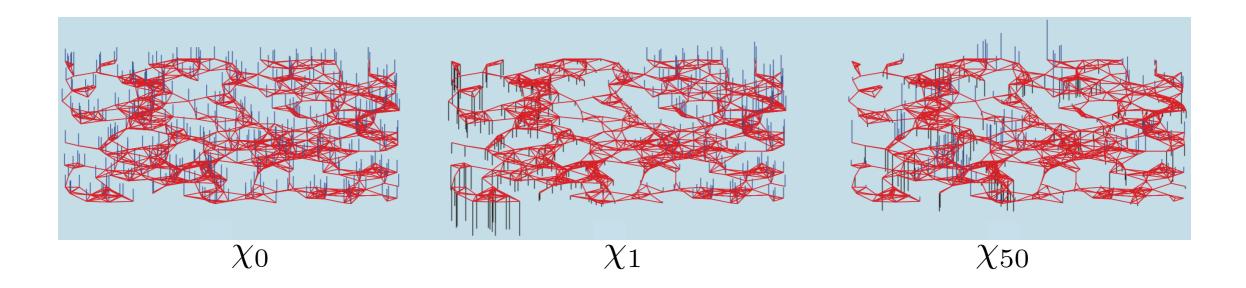
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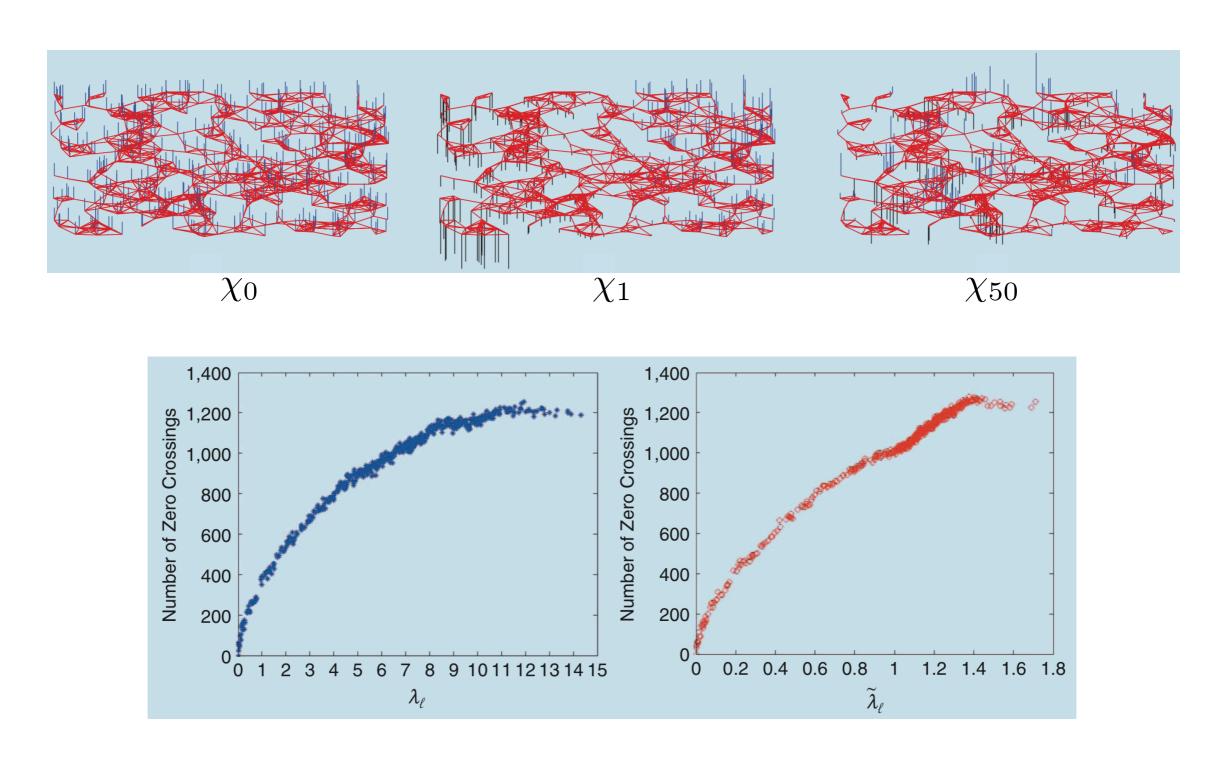
$$\chi \qquad \qquad \Lambda \qquad \qquad \chi^T$$

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

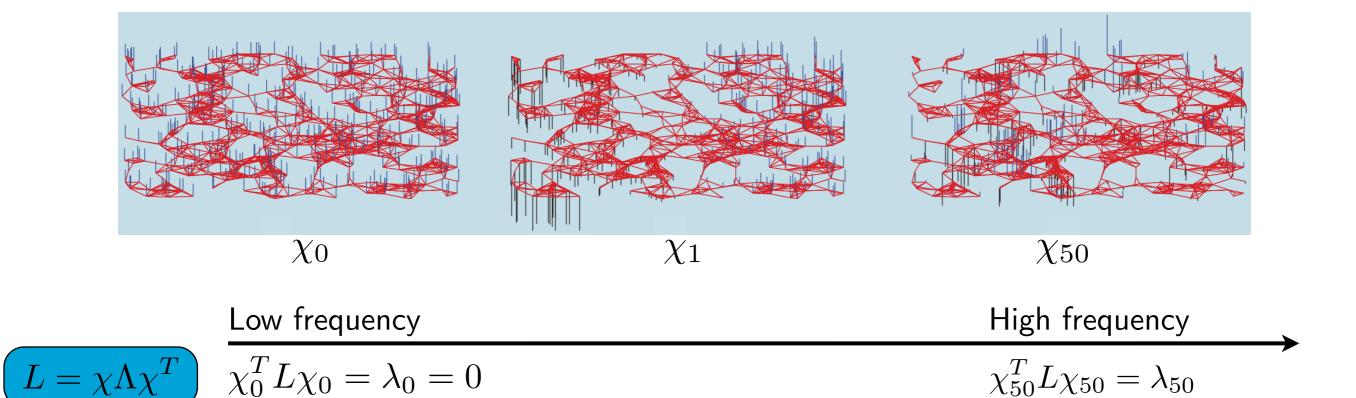
## Graph Fourier transform



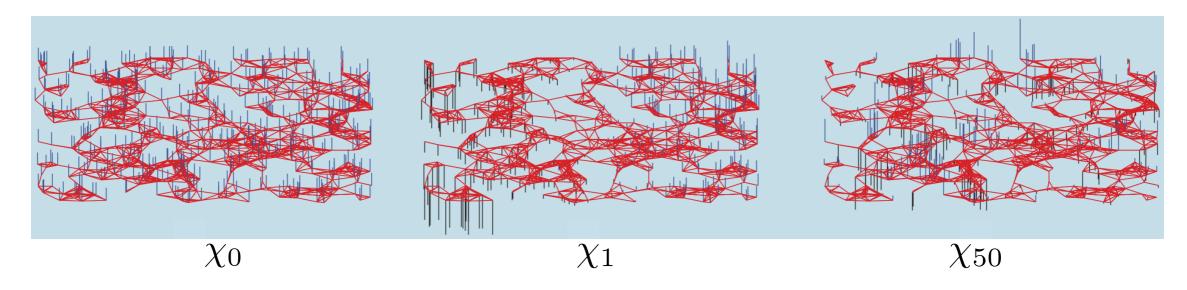
## Graph Fourier transform



#### Graph Fourier transform



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



Low frequency

High frequency

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

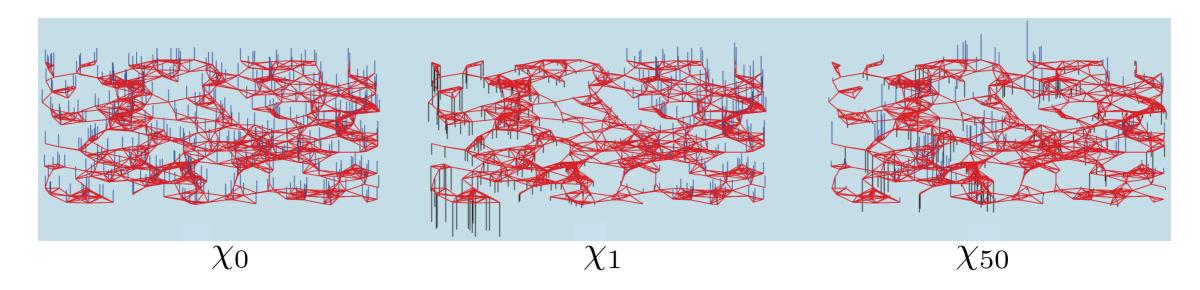
$$\left(L = \chi \Lambda \chi^T\right) \quad \chi_0^T L \chi_0 = \lambda_0 = 0$$

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

#### **Graph Fourier transform:**

[Hammond11]

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



Low frequency

High frequency

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

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:

$$\hat{f}(\ell) = \langle \chi_\ell, f \rangle : \begin{bmatrix} 1 & 1 & 1 \\ \chi_0 & \cdots & \chi_{N-1} \end{bmatrix}^T \int_{\lambda_0 \lambda_1 \ \lambda_2 \ \lambda_3 \ \lambda_4 \ \cdots \ \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_2 \lambda_3 \lambda_4 \cdots \lambda_{N-1}} \int_{\text{Low frequency}} \frac{1}{\lambda_0 \lambda_1 \lambda_2 \lambda_2 \lambda_3 \lambda_4 \cdots$$

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

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one-dimensional Laplace operator:  $abla^2$ 



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



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

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

The Laplacian L admits the following eigendecomposition:  $L\chi_{\ell} = \lambda_{\ell}\chi_{\ell}$ 

one-dimensional Laplace operator:  $-\nabla^2$  : graph Laplacian: L



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eigenvectors:  $\chi_\ell$ 

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

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 Classical FT: 
$$\hat{f}(\omega)=\int{(e^{j\omega x})^*f(x)dx}$$
 Graph FT: 
$$\hat{f}(\ell)=\langle\chi_\ell,f\rangle=\sum_{i=1}^N\chi_\ell^*(i)f(i)$$

$$f(i) = \sum_{\ell=0}^{N-1} \hat{f}(\ell) \chi_{\ell}(i)$$

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



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

$$f(x) = \frac{1}{2\pi} \int \hat{f}(\omega) e^{j\omega x} d\omega \qquad \qquad f(i) = \sum_{\ell=0}^{N-1} \hat{f}(\ell) \chi_{\ell}(i)$$



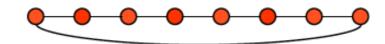
eigenvectors:  $\chi_\ell$ 

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

Classical FT: 
$$\hat{f}(\omega) = \int e^{j\omega x} f(x) dx$$
 Graph FT:  $\hat{f}(\ell) = \langle \chi_{\ell}, f \rangle = \sum_{i=1}^{N} \chi_{\ell}^{*}(i) f(i)$ 

$$f(i) = \sum_{\ell=0}^{N-1} \hat{f}(\ell) \chi_{\ell}(i)$$

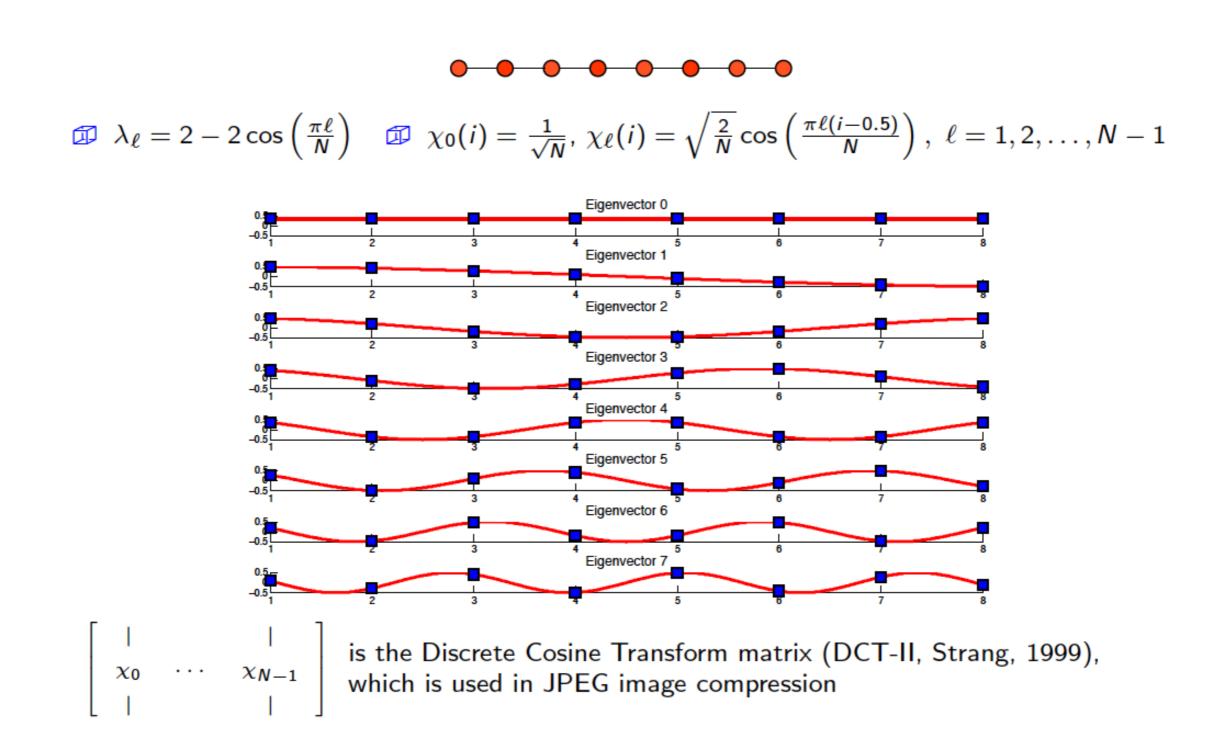
## Two special cases



- (Unordered) Laplacian eigenvalues:  $\lambda_\ell = 2 2\cos\left(\frac{2\ell\pi}{N}\right)$
- One possible choice of orthogonal Laplacian eigenvectors:

$$\chi_{\ell} = \left[1, \omega^{\ell}, \omega^{2\ell}, \dots, \omega^{(N-1)\ell}\right], \text{ where } \omega = e^{\frac{2\pi j}{N}}$$

## Two special cases



### Outline

- Motivation
- Graph signal processing (GSP): Basic concepts
- Spectral filtering: Basic tools of GSP
- Connection with literature
- Applications in neuroscience

# Classical frequency filtering

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

# Classical frequency filtering

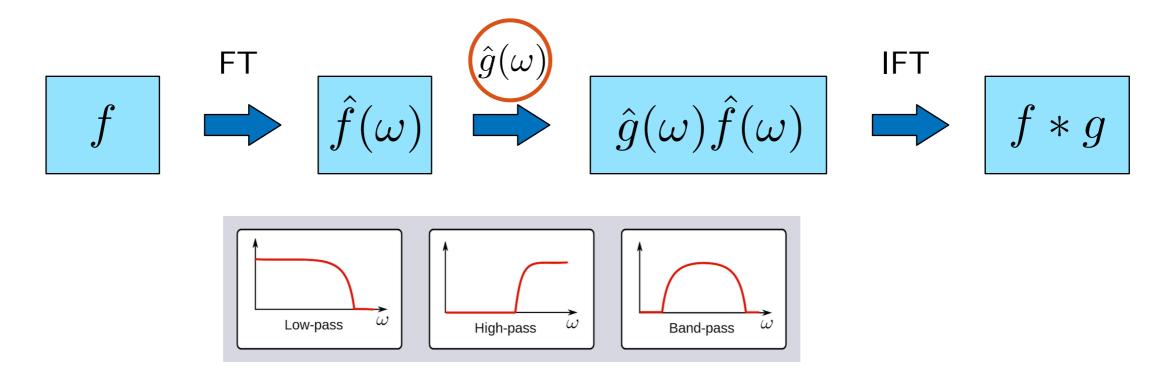
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Apply filter with transfer function  $\hat{g}(\cdot)$  to a signal f

# Classical frequency filtering

Classical FT: 
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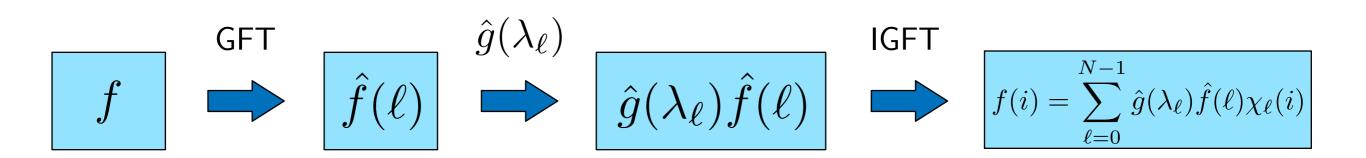
Apply filter with transfer function  $\hat{g}(\cdot)$  to a signal f



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

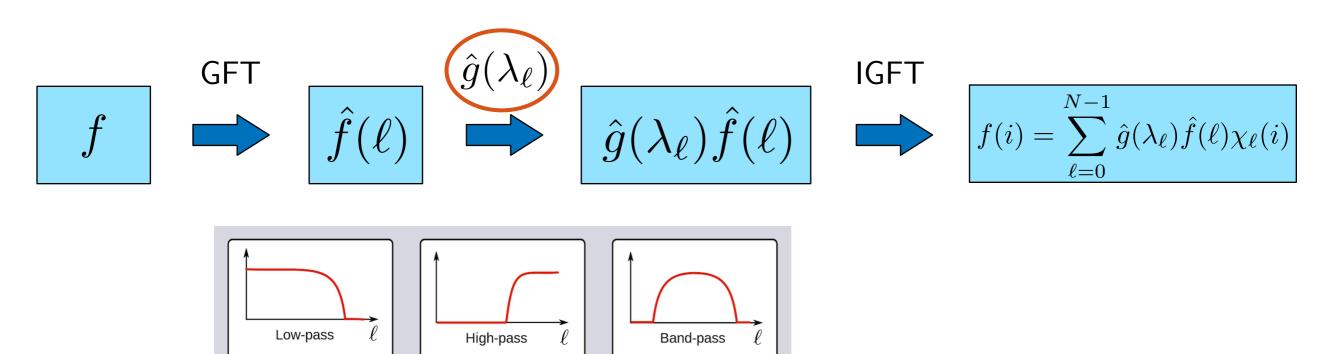
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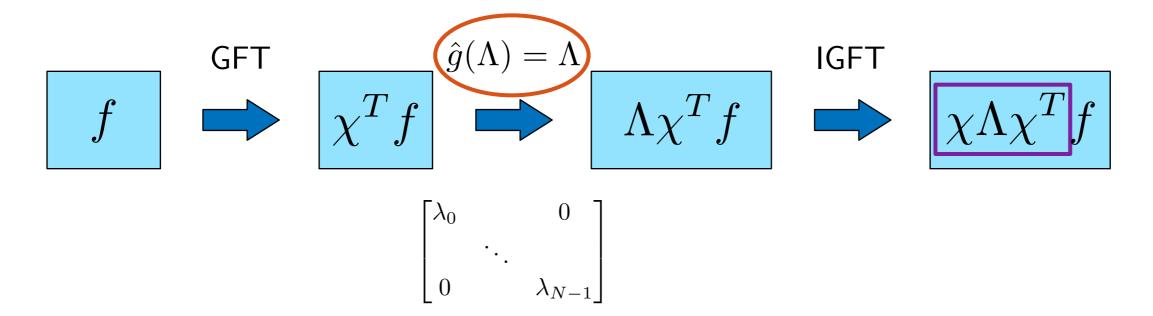
$$f \qquad \widehat{g}(\Lambda) \qquad \widehat{g}(\Lambda) \chi^T f \qquad \widehat{g}(\Lambda) \chi^T f$$

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

## Graph Laplacian revisited

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

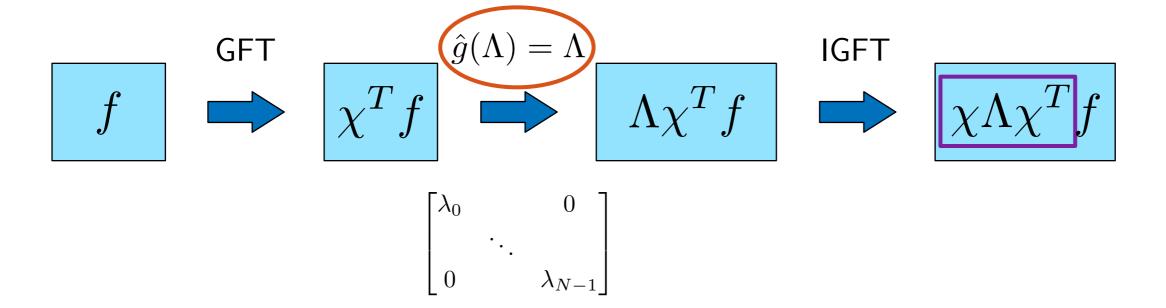
The Laplacian L is a difference operator:  $Lf = \chi \Lambda \chi^T f$ 



## Graph Laplacian revisited

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

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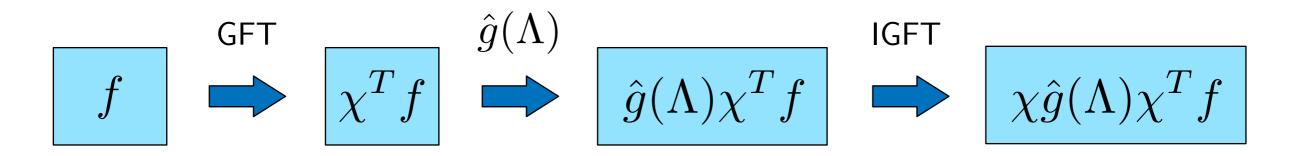


The Laplacian operator filters the signal in the spectral domain by its eigenvalues!

The Laplacian quadratic form:  $f^T L f = ||L^{\frac{1}{2}} f||_2 = ||\chi \Lambda^{\frac{1}{2}} \chi^T f||_2$ 

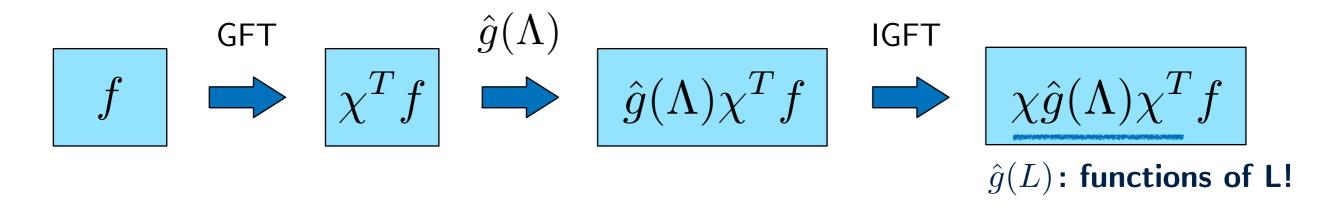
# Graph transform/dictionary design

 Transforms and dictionaries can be designed through graph spectral filtering: Functions of graph Laplacian!



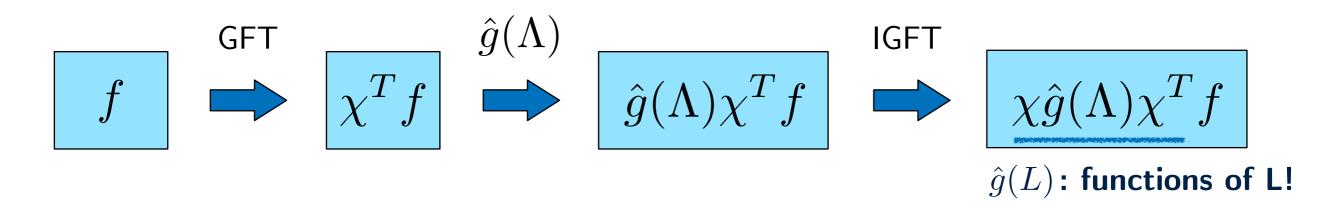
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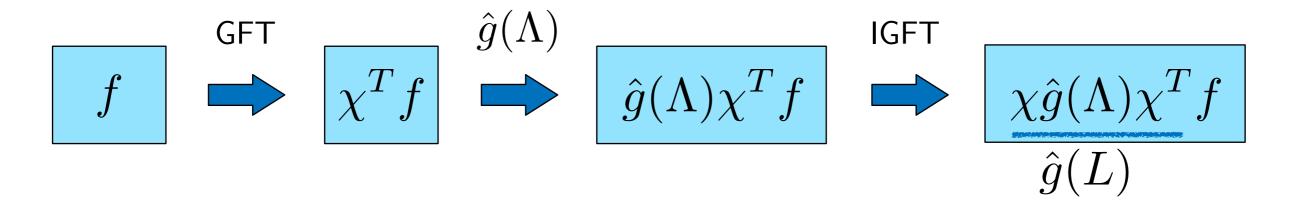


# Graph transform/dictionary design

 Transforms and dictionaries can be designed through graph spectral filtering: Functions of graph Laplacian!



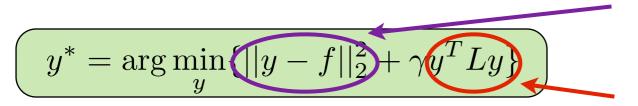
- Important properties can be achieved by properly defining  $\hat{g}(L)$  , such as localisation of atoms
- Closely related to kernels and regularisation on graphs



Problem: We observe a noisy graph signal  $f = y_0 + \eta$  and wish to recover  $y_0$ 

$$y^* = \arg\min_{y} \{ ||y - f||_2^2 + \gamma y^T L y \}$$

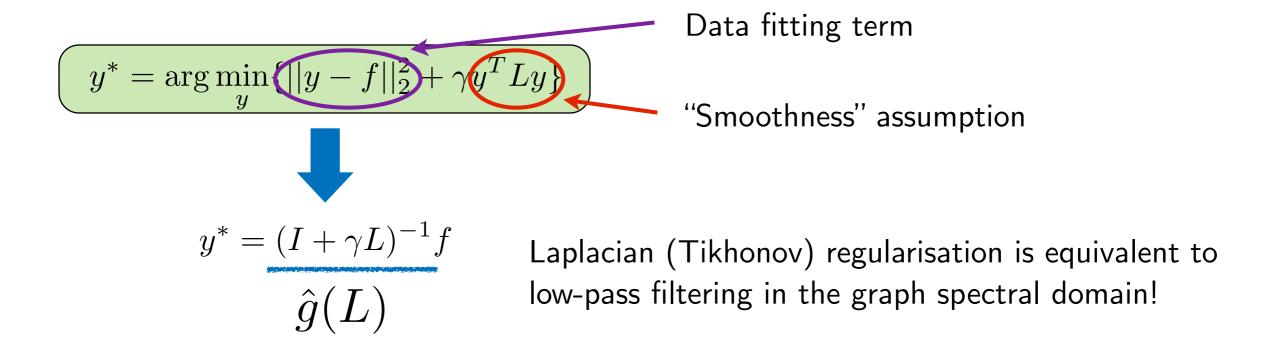
Problem: We observe a noisy graph signal  $f = y_0 + \eta$  and wish to recover  $y_0$ 



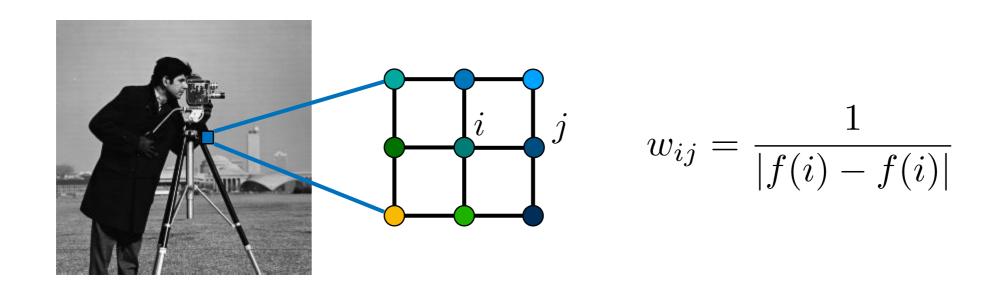
Data fitting term

"Smoothness" assumption

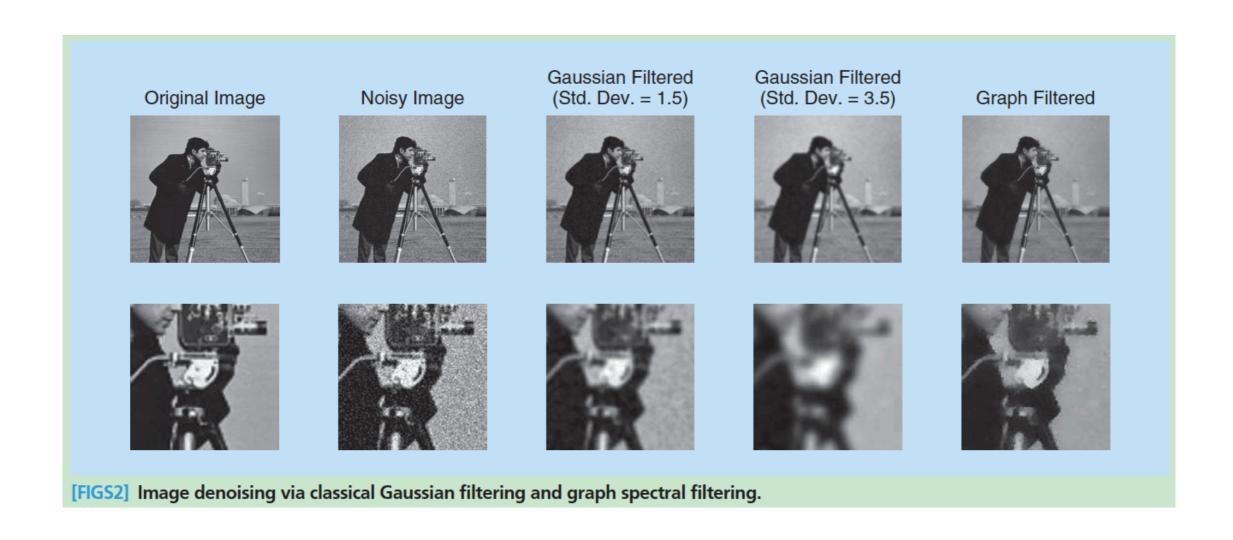
Problem: We observe a noisy graph signal  $f = y_0 + \eta$  and wish to recover  $y_0$ 



- noisy image as the observed noisy graph signal
- regular grid graph (weights inversely proportional to pixel value difference)



- noisy image as the observed noisy graph signal
- regular grid graph (weights inversely proportional to pixel value difference)



## Example designs

Low-pass filters:  $\hat{g}(L) = (I + \gamma L)^{-1} = \chi (I + \gamma \Lambda)^{-1} \chi^T$ 

## Example designs

$$\begin{array}{c|c} & \widehat{g}(\Lambda) \\ \hline f & & & \widehat{g}(\Lambda) \\ \hline & & & & \widehat{g}(\Lambda)\chi^T f \\ \hline & & & & \widehat{g}(\Lambda)\chi^T f \\ \hline & & & & & \widehat{g}(L) \\ \hline \end{array}$$

Low-pass filters: 
$$\hat{g}(L) = (I + \gamma L)^{-1} = \chi (I + \gamma \Lambda)^{-1} \chi^T$$

Window kernel: Windowed graph Fourier transform

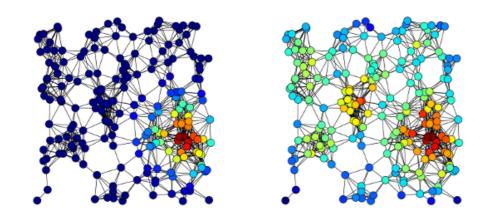
Shifted and dilated band-pass filters: Spectral graph wavelets  $\hat{g}(sL)$ 

Adapted kernels: Learn values of  $\hat{g}(L)$  directly from data

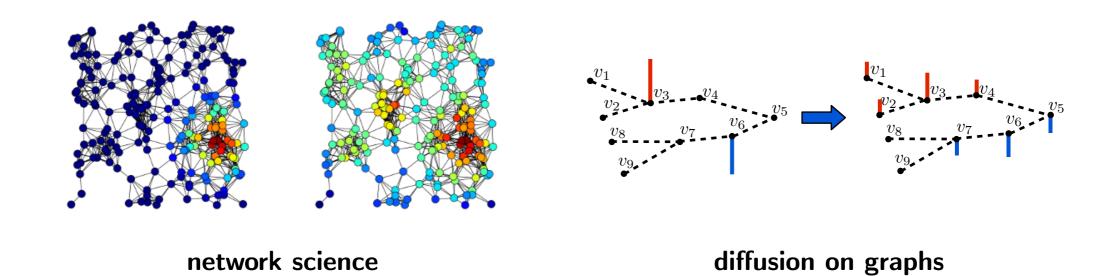
Parametric polynomials: 
$$\hat{g}_s(L) = \sum_{k=0}^K \alpha_{sk} L^k = \chi(\sum_{k=0}^K \alpha_{sk} \Lambda^k) \chi^T$$

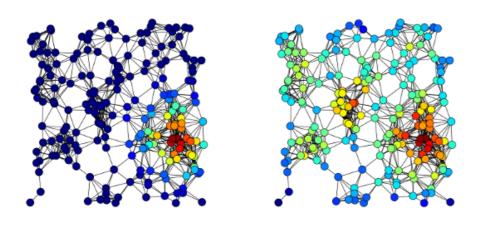
### Outline

- Motivation
- Graph signal processing (GSP): Basic concepts
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- Connection with literature
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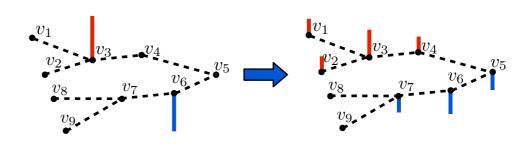


network science

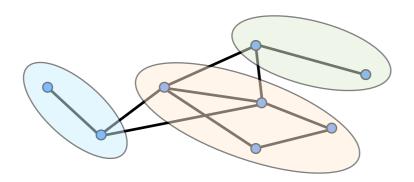




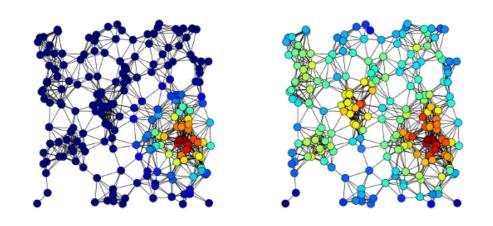
network science



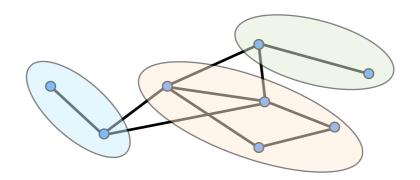
diffusion on graphs



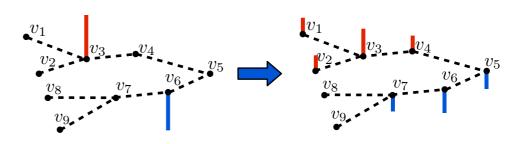
unsupervised learning (dimensionality reduction, clustering)



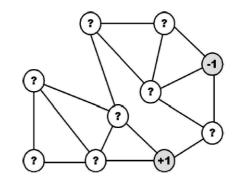
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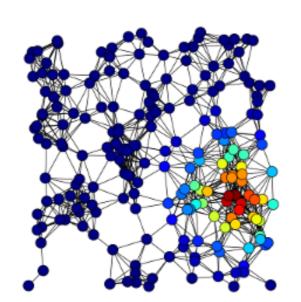
diffusion on graphs



semi-supervised learning

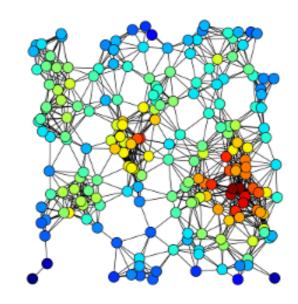
# Network centrality

#### eigenvector centrality



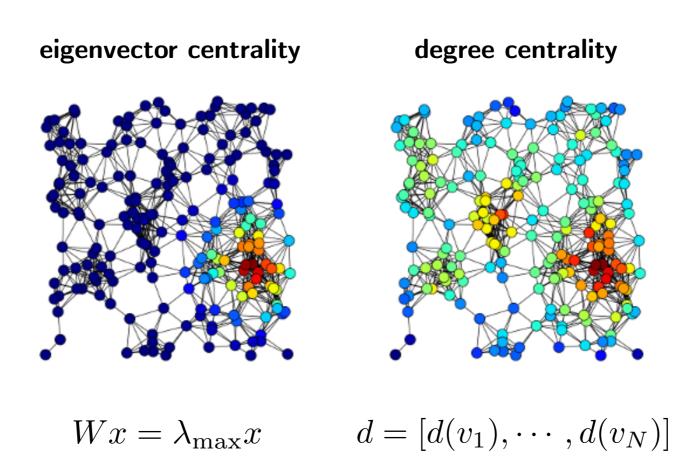
$$Wx = \lambda_{\max} x$$

#### degree centrality



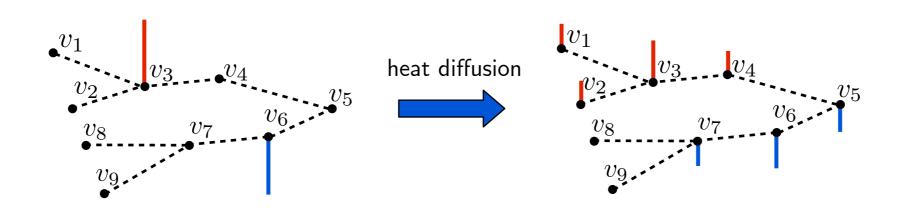
$$Wx = \lambda_{\max} x$$
  $d = [d(v_1), \cdots, d(v_N)]$ 

# Network centrality

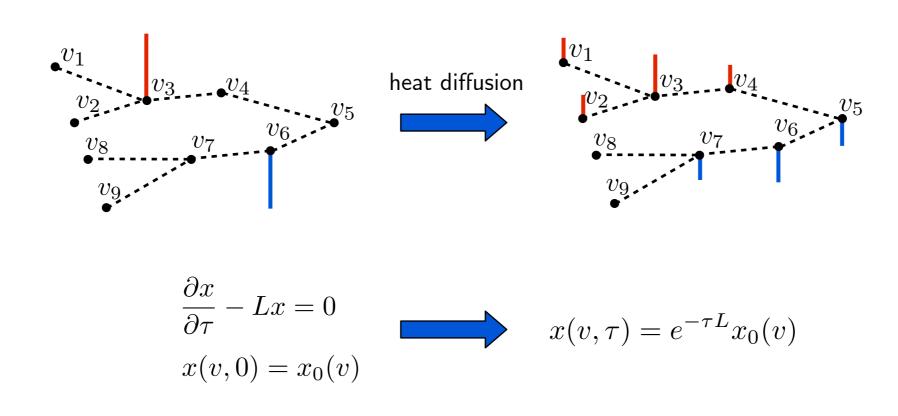


- Google's PageRank is a variant of eigenvector centrality
- eigenvectors of W can also be used to provide a frequency interpretation for graph signals

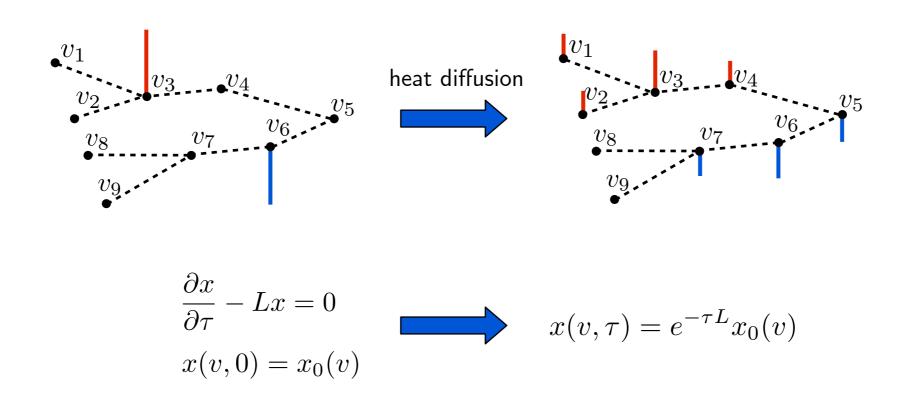
# Diffusion on graphs



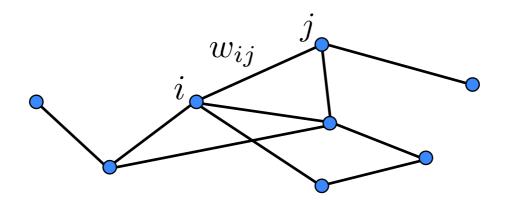
# Diffusion on graphs

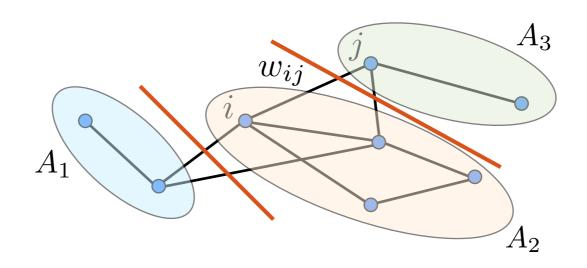


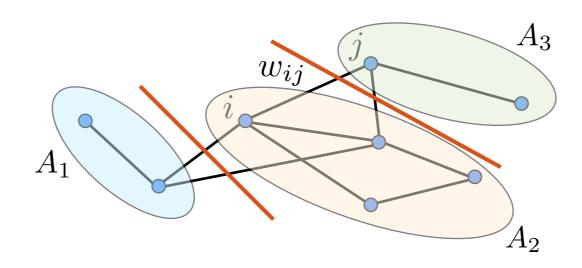
# Diffusion on graphs



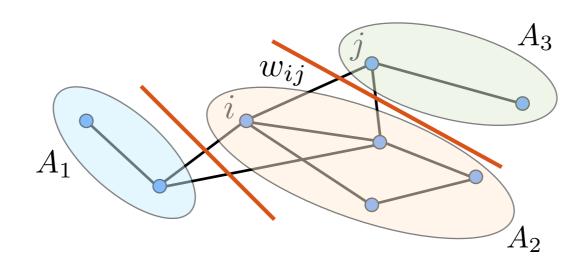
- heat diffusion on graphs is a typical physical process on graphs
- other possibilities exist (e.g., random walk on graphs)
- many have an interpretation of filtering on graphs







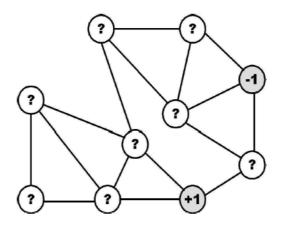
$$NCut(A_1, ..., A_k) = \frac{1}{2} \sum_{i=1}^{k} \frac{W(A_i, \overline{A_i})}{vol(A_i)}$$



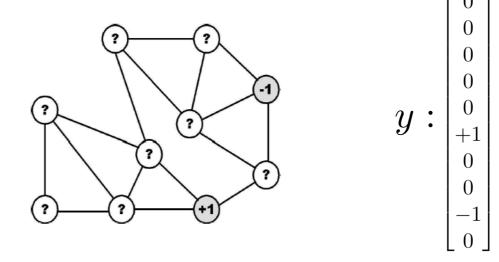
$$NCut(A_1, ..., A_k) = \frac{1}{2} \sum_{i=1}^{k} \frac{W(A_i, \overline{A_i})}{vol(A_i)}$$

- first k eigenvectors of graph Laplacian minimise the graph cut
- eigenvectors of graph Laplacian enable a Fourier-like analysis for graph signals

# Semi-supervised learning

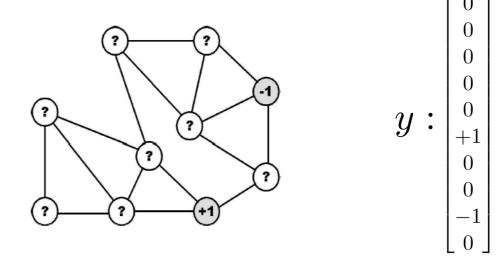


# Semi-supervised learning



$$\min_{x \in \mathbb{R}^N} ||y - x||_2^2 + \alpha \ x^T L x,$$

# Semi-supervised learning

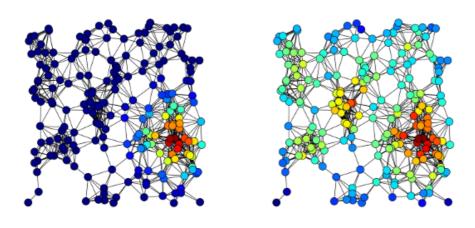


$$\min_{x \in \mathbb{R}^N} ||y - x||_2^2 + \alpha \ x^T L x,$$

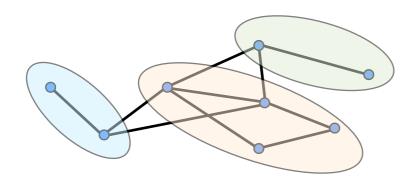
- learning by assuming smoothness of predicted labels
- this is equivalent to a denoising problem for graph signal y

#### GSP and the literature

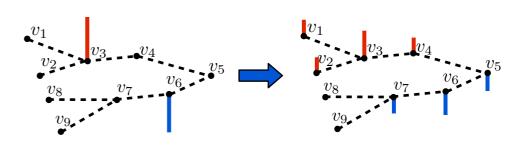
centrality, diffused information, class membership, node labels (and node-level features in general) can ALL be viewed as graph signals



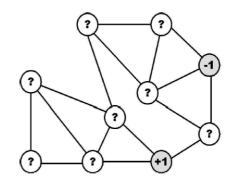
network science



unsupervised learning (dimensionality reduction, clustering)



network diffusion

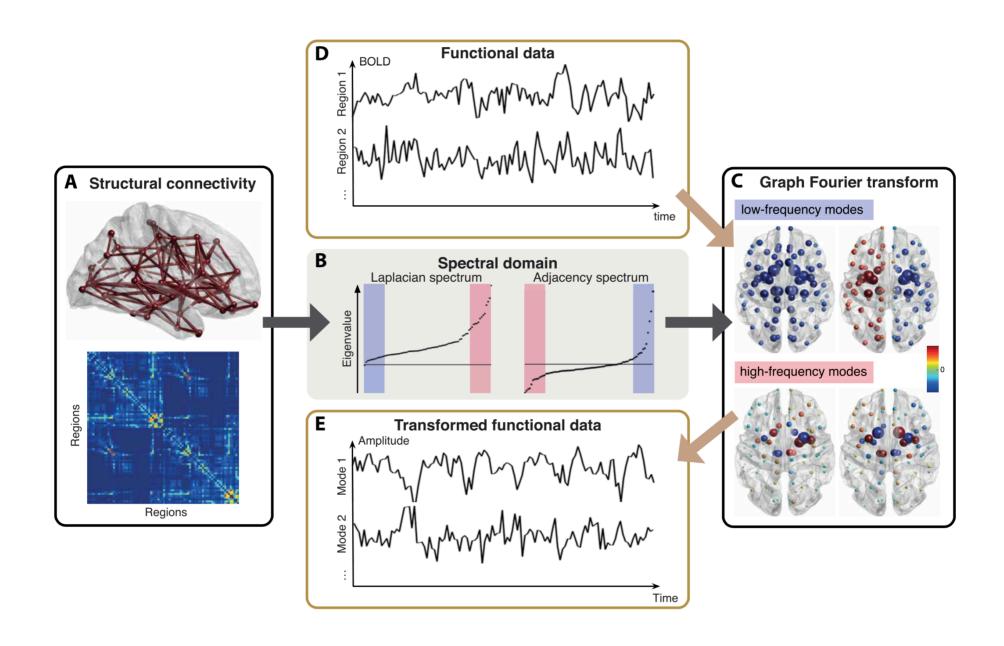


semi-supervised learning

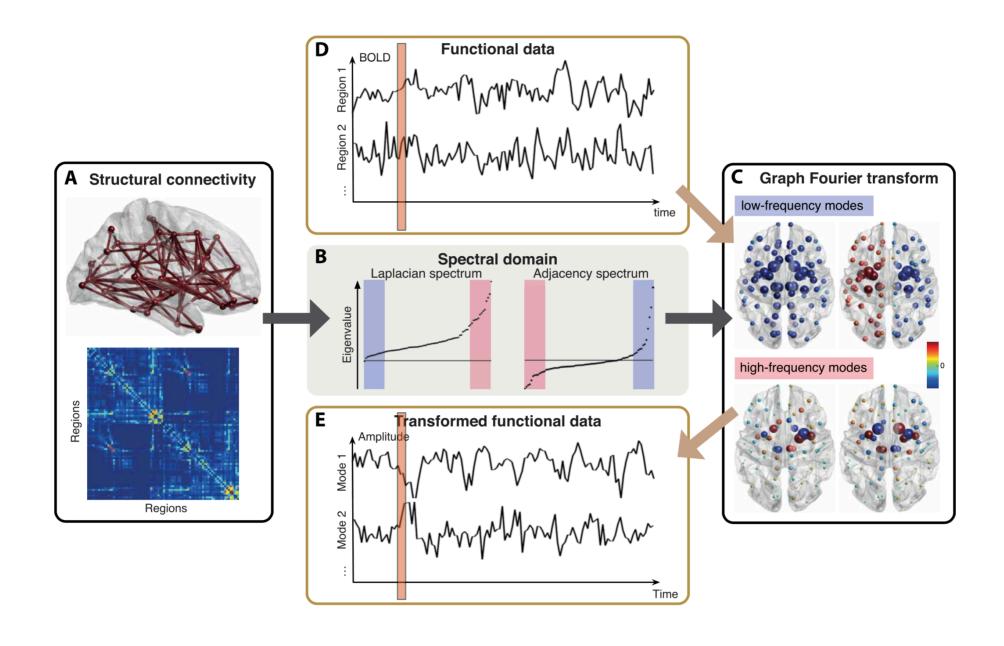
#### Outline

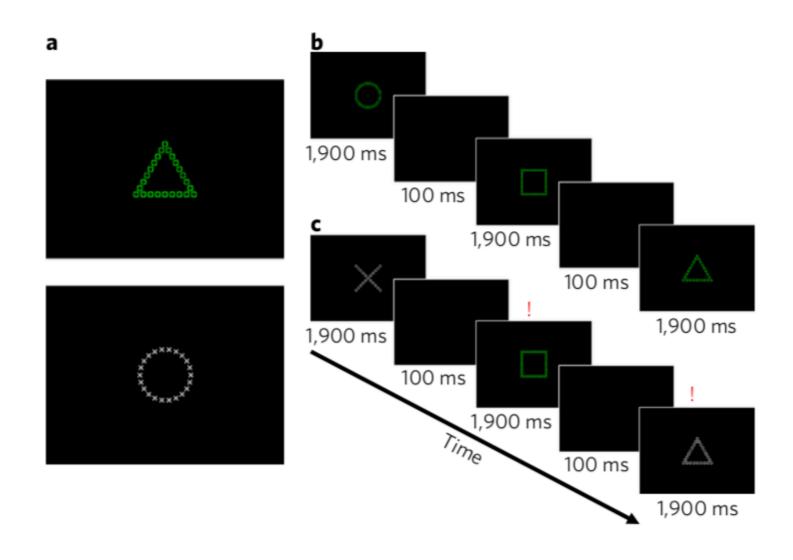
- Motivation
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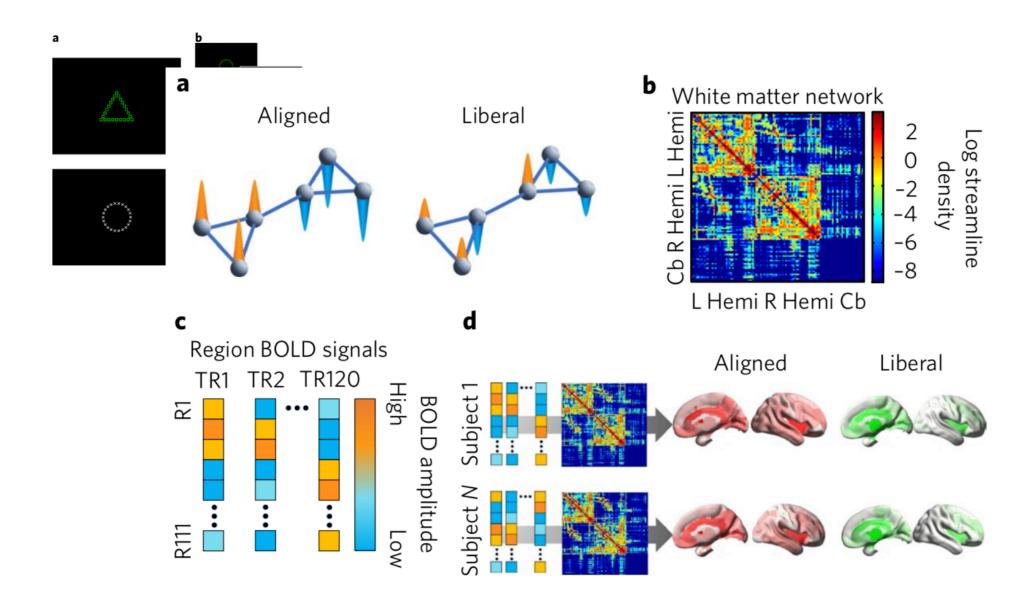
### A typical analysis framework

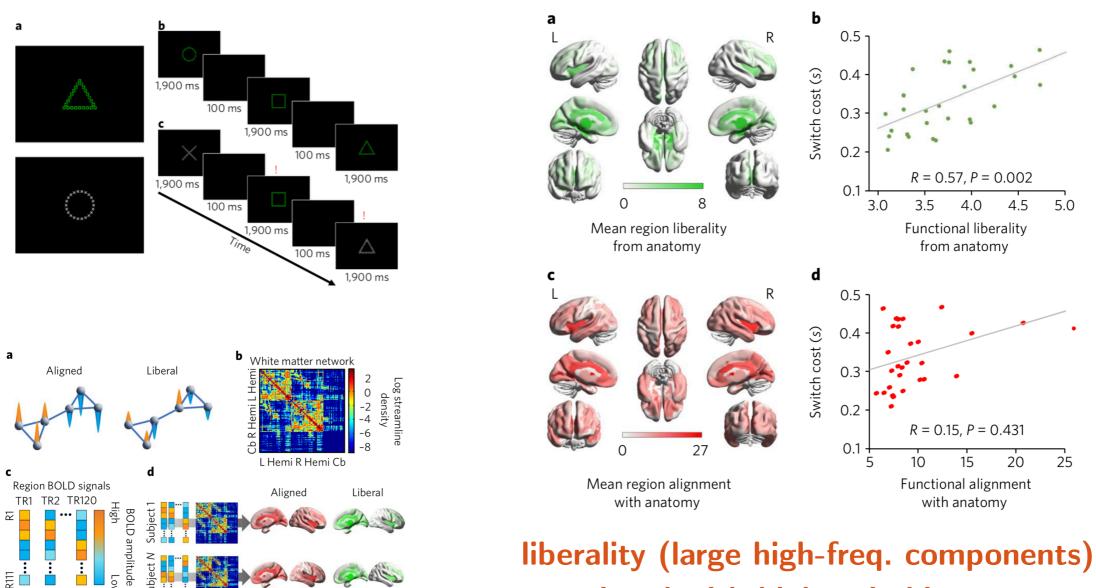


### A typical analysis framework







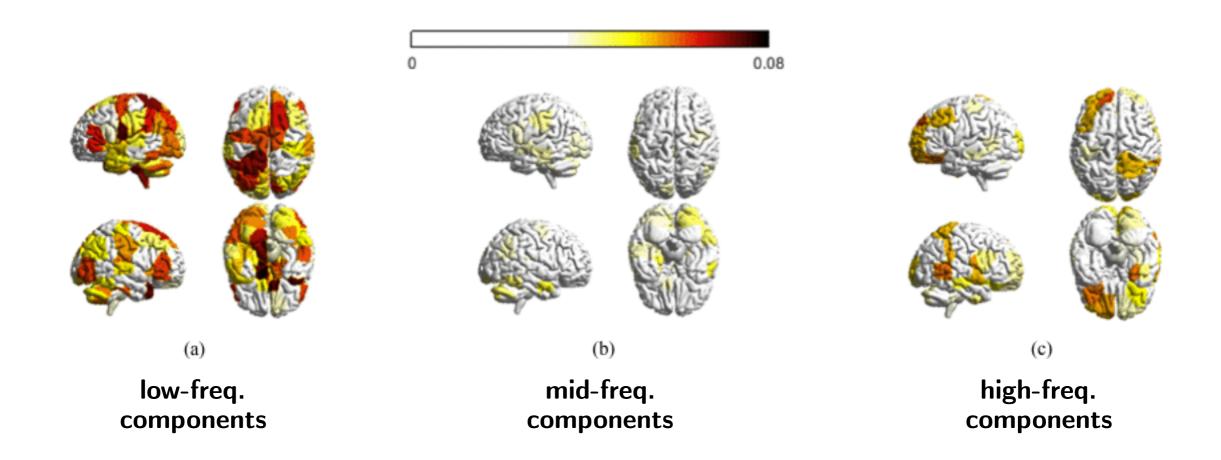


associated with high switching cost

Medaglia et al., "Functional alignment with anatomical networks is associated with cognitive flexibility", Nature Human Behaviour, 2018.

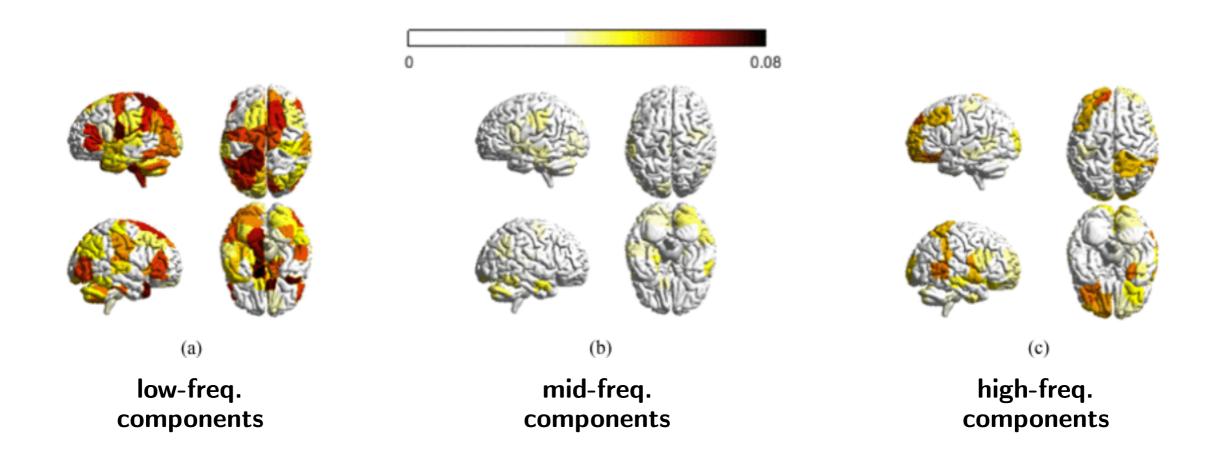
5.0

25

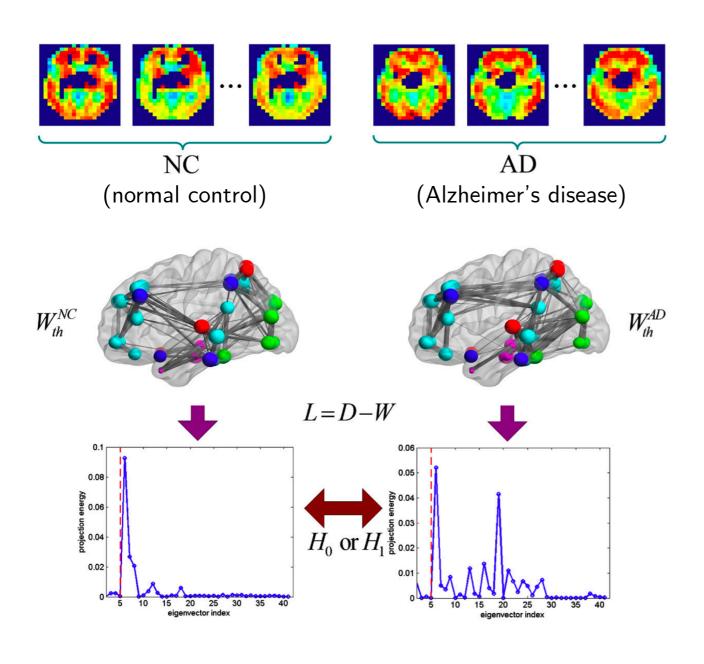


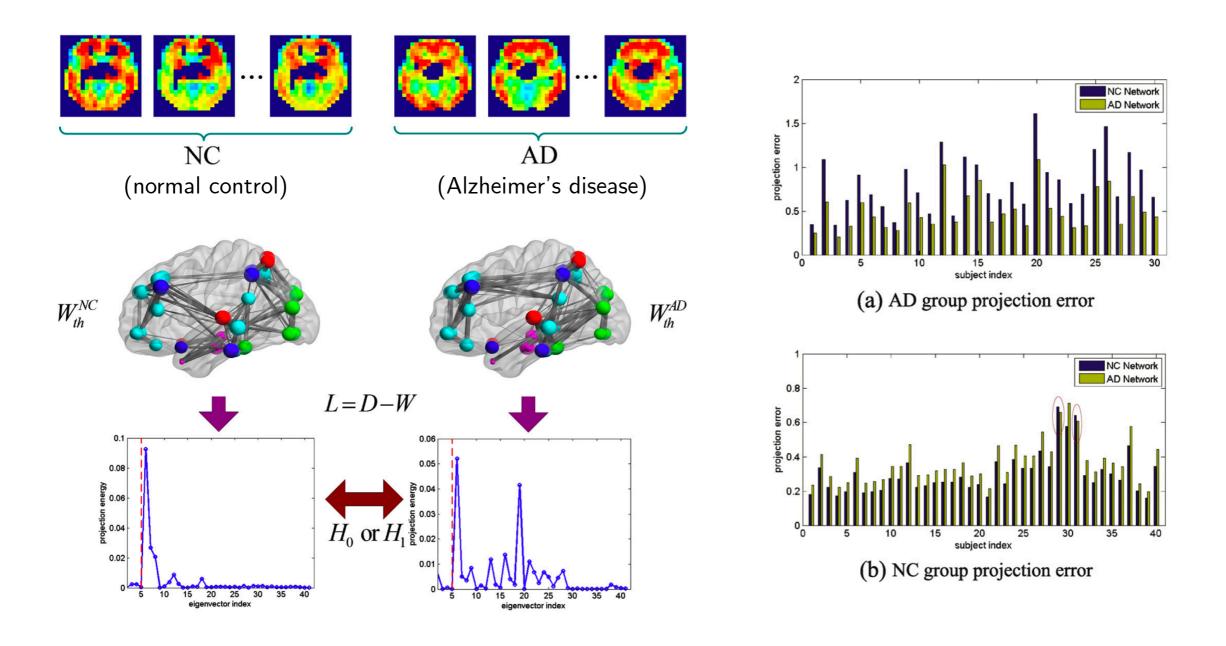
- record BOLD signals while responding to sequentially presented stimuli

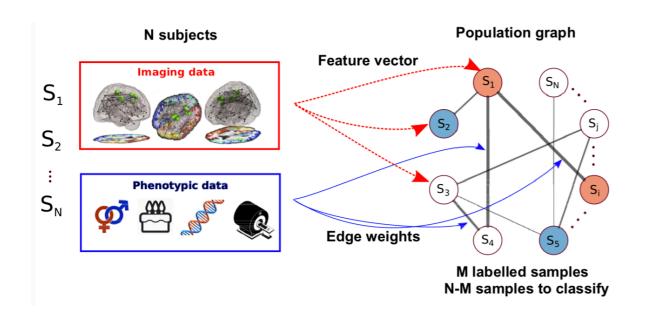
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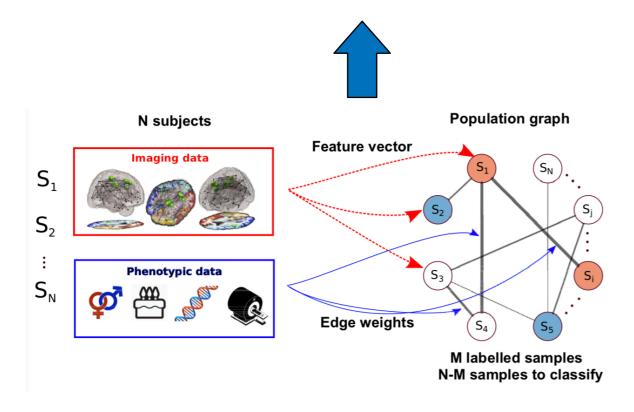
- record BOLD signals while responding to sequentially presented stimuli
- it favours learning to have
  - smooth, spread signals (low-freq.) when facing unfamiliar task
  - varied, spiking signals (high-freq.) when task becomes familiar



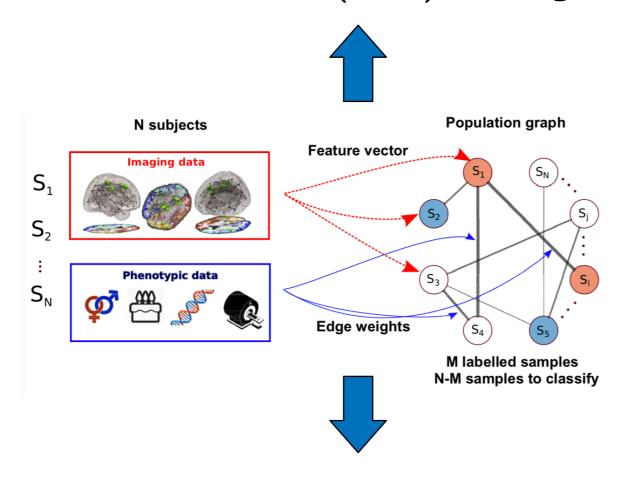




ADNI (structural MRI): volumes of brain structures ABIDE (fMRI): off-diagonal of functional connectivity

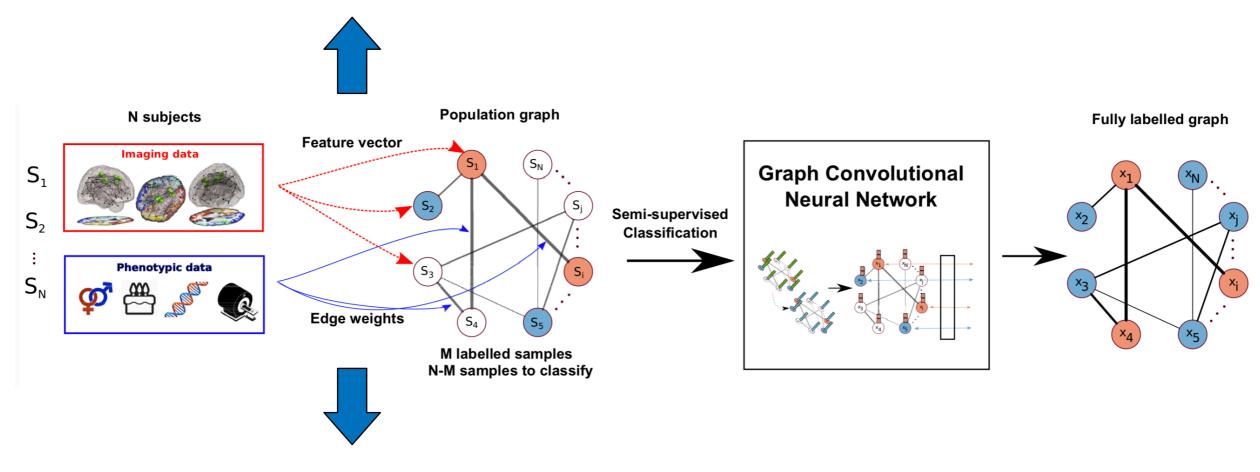


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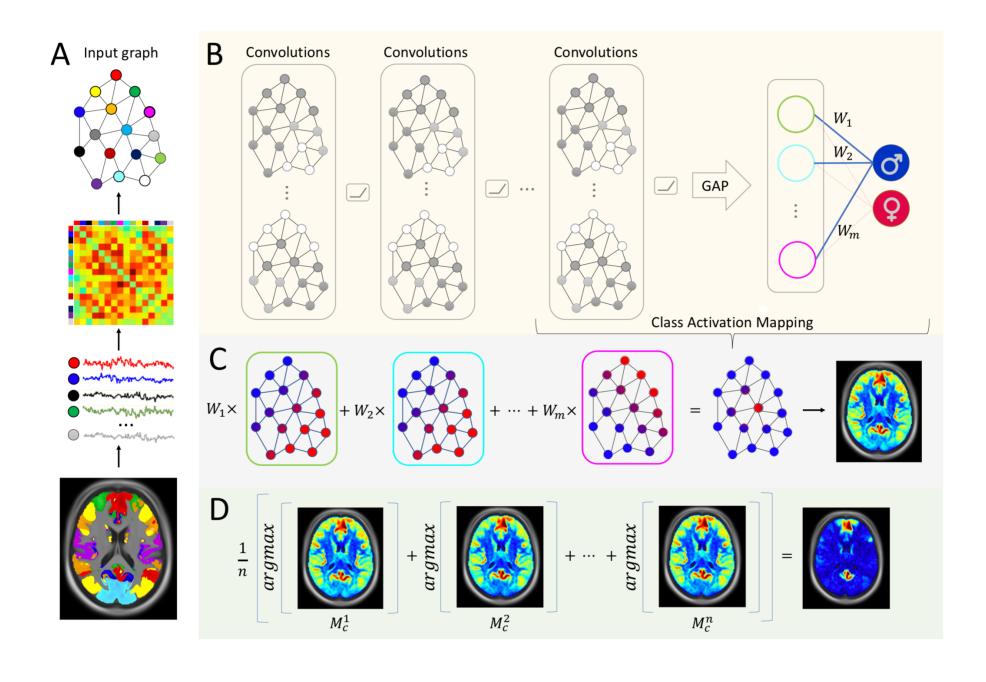
similarity in phenotypic data

ADNI (structural MRI): volumes of brain structures ABIDE (fMRI): off-diagonal of functional connectivity

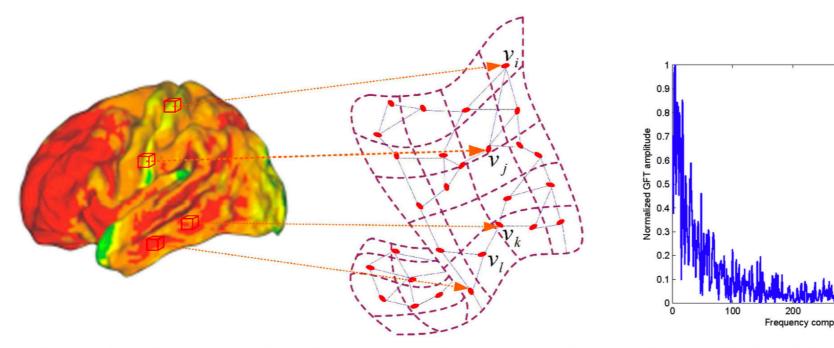


similarity in phenotypic data

# Application III: Gender classification



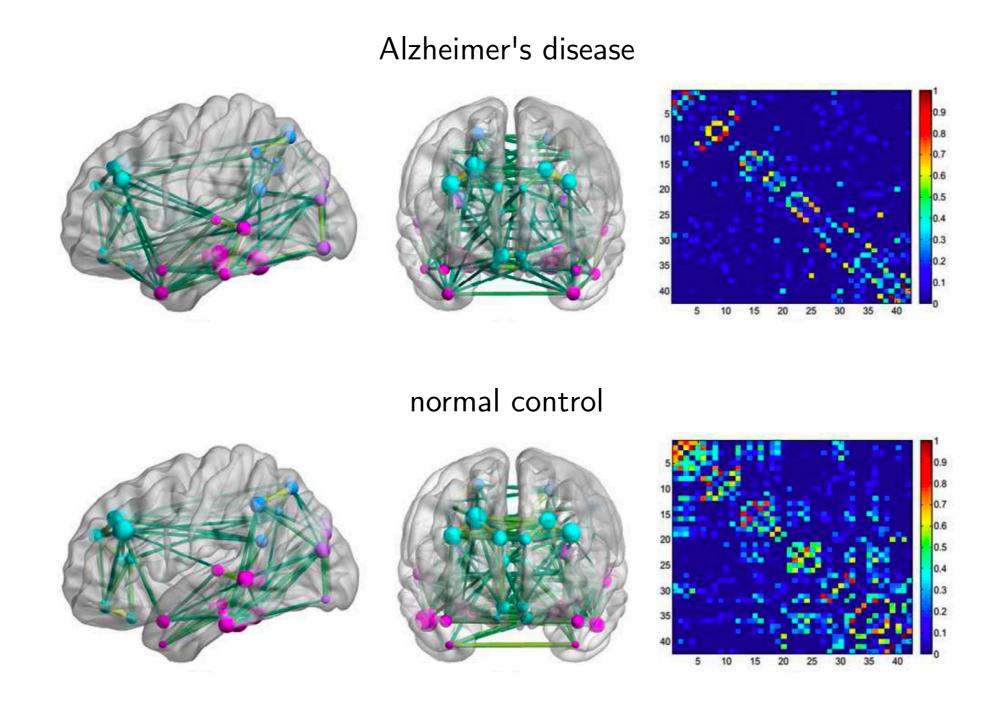
# Application IV: Inferring brain connectivity



(a) Mapping from image voxels (cubes) to vertices (ellipses) of a graph. (b) Amplitudes of the GFT coefficients.

Hu et al., "A spectral graph regression model for learning brain connectivity of Alzheimer's disease", PLOS ONE, 2015. Shen et al., "Nonlinear structural vector autoregressive models for inferring effective brain network connectivity", 2016.

# Application IV: Inferring brain connectivity



Hu et al., "A spectral graph regression model for learning brain connectivity of Alzheimer's disease", PLOS ONE, 2015. Shen et al., "Nonlinear structural vector autoregressive models for inferring effective brain network connectivity", 2016.

#### Future of GSP

- Mathematical models for graph signals
  - global and local smoothness / regularity
  - underlying physical processes
- Graph construction
  - how to infer topologies given observed data?
- Fast implementation
  - fast graph Fourier transform
  - distributed processing
- Connection to / combination with other fields
  - statistical machine learning
  - deep learning on graphs and manifolds
- Key applications

#### Resources

Three tutorial/overview papers:

David I Shuman, Sunii K. Narang, Pascal Frossard, Antonio Ortega, and Pierre Vandergheynst

#### The Emerging Field of Signal Processing on Graphs



Extending high-dimensional data analysis to networks and other irregular domains

n applications such as social, energy, transportation, sensor, and neuronal networks, high-dimensional data naturally reside on the vertices of weighted graphs. The emerging field of signal processing on graphs merges algebraic and spectral graph theoretic concepts with computational harmonic analysis to process such signals on graphs. In this tutorial overview, we outline the main challenges of the area, discuss different ways to define nearboard developed which we the analysis of the second developed to graph theoretic concepts with computational harmonic anal-ysis to process such signals on graphs. In this tutorial overview, we cuttlie the main challenges of the area, discuss different ways to define graph spectral domains, which are the analogs to the classical frequency domain, and highlight the importance of the classical frequency domain, and highlight the importance of

classical frequency domain, and highlight the importance of incoporating the irregular structures of graph data domains with the irregular structures of graph data domains with the processing signals on graphs. We then review methods to generalize fundamental operations such as filtering, translation, modulation, dislation, and downsampling to the graph setting and survey the localized, multiscale transforms that have except the property of the physical distance weight may be inversely proportional to the physical distance contains the network. The data for these creates in the network. between the two vertices it connects. The connectivities and edge weights are either dictated by the physics of the problem at hand or inferred from the data. For instance, the edge weight may be inversely proportional to the physical distance between nodes in the network. The data on these graphs can be visualized as a finite collection of samples, with one sample at each vertex in the graph. Collectively, we refer to these



#### **Graph Signal Processing:** Overview, Challenges, and Applications

This article presents methods to process data associated to graphs (graph signals) extending techniques (transforms, sampling, and others) that are used for conventional signals.

By Antonio Ortega<sup>®</sup>, Fellow IEEE, Pascal Frossard, Fellow IEEE, Jelena Kovačević, Fellow IEEE, José M. F. Moura<sup>®</sup>, Fellow IEEE, and Pierre Vandergheynst

AISTRACT | Research in graph signal processing (6GP) aims to develop tools for processing data defined on irregular graph domains. In this paper, we first provide an overview of one-likean in GSP and their connection to conventional digital signal processing, along with a brief historical perspective to highlight how concepts recently developed in GSP build on top of prior research in other areas. We then commaries recent advance in developing basic GSP books on the control of the

I. INTRODUCTION AND MOTIVATION
Data is all around us, and mastive amounts of it. Almost
every aspect of human life is now being recorded at all levell: from the marking and recording of processing inside the
cells tarting with the advent of fluorescent markers, to our
personal data through health monitoring devices and appe,
financial and banking data, our social networks, mobility
and traffic pattern, marketing preferences, faids, and many
more. The complexity of such networks [1] and interactions
meant that the data now reside on irregular and complex
structures that do not lend themselves to trandard tools.

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gathered in the classical setting and extend it to graphs; we can talk about the notions of frequency and bandlimitedness,

#### A Graph Signal Processing Perspective on Functional **Brain Imaging**

This article addresses how the signal processing view on brain graphs can provide additional insights into brain network analysis.

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analyze the signals from a new viewpoint. Here, we review GSP for brain imaging data and discuss their potential to integrate brain structure and function; i.e., how the brain is wired, and where and when activity takes place. Data acquired using these techniques can be analyzed in terms of its network structure toreveal organizing-principles at the systems level. Graph representations are versatile models where nodes are associated to brain regions and edges to structural or functional connections. are the anatomical backbone between regions. Functional graphs are built based on functional connectivity, which is a pairwise measure of statistical interdependence between the control of the control measure of statistical interdependency between pairs of regional activity traces. Therefore, most research to date has focused on analyzing these graphs reflecting structure or function. Graph signal processing (GSP) is an emerging area of research where signals recorded at the nodes of the graph are studied atop the underlying graph structure. An increasing number of fundamental operations have been generalized to the graph setting, allowing to

sive manner [2]. Diffusion-weighted MRI allows to measure major fiber tracts in white matter and thereby map the structural scaffold that supports neural communication. Functional MRI (fMRI) takes an indirect estimate of the brain approximately each second, in the form of blood oxy-genation level-dependent (BOLD) signals. An emerging theme in computational neuroimaging is to study the brain at the systems level with such fundamental questions as how it

ity patterns that often look haphazard yet are crucial in ry patterns that often look haphazard yet are crucial in cognitive processes. The apparent importance of these con-nectomes has motivated the emergence of network neuro-science as a clearly defined field to study the relevance of

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