Graph signal processing

Concepts, tools and applications

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Outline

- Motivation
- Graph signal processing (GSP): Basic concepts
- Spectral filtering: Basic tools of GSP
- Applications and perspectives

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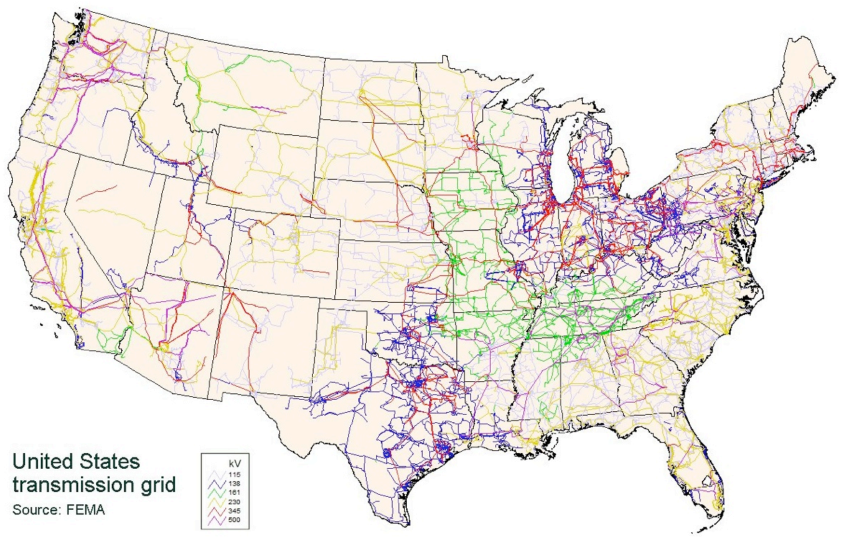
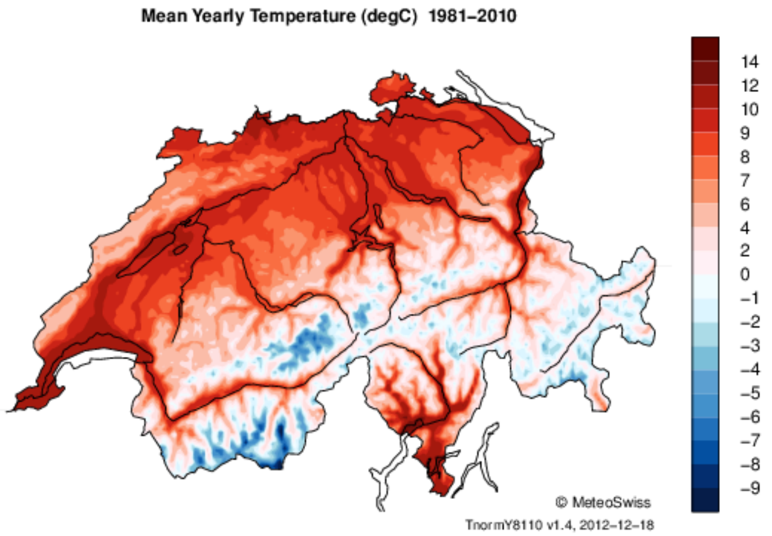
Data are often structured

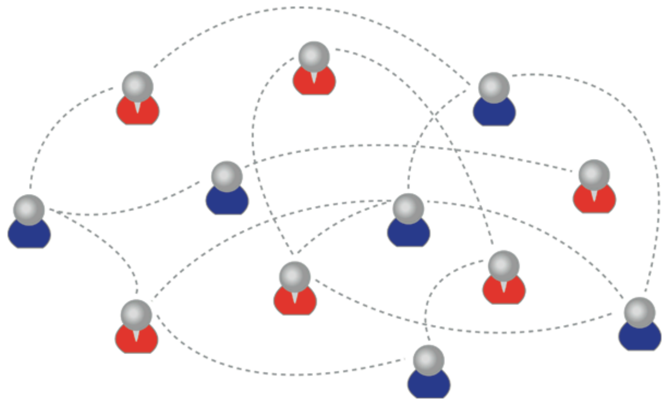


Electrical data

Traffic data

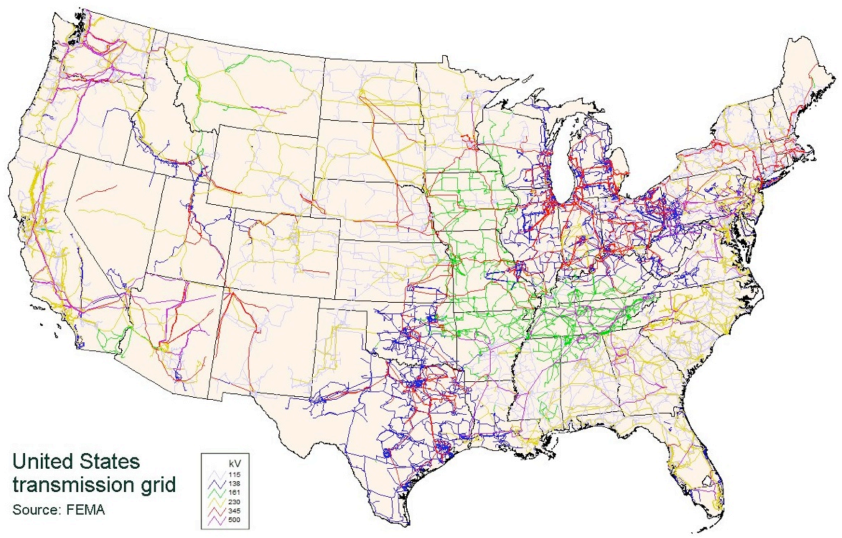


Temperature data



Social network data

Data are often structured



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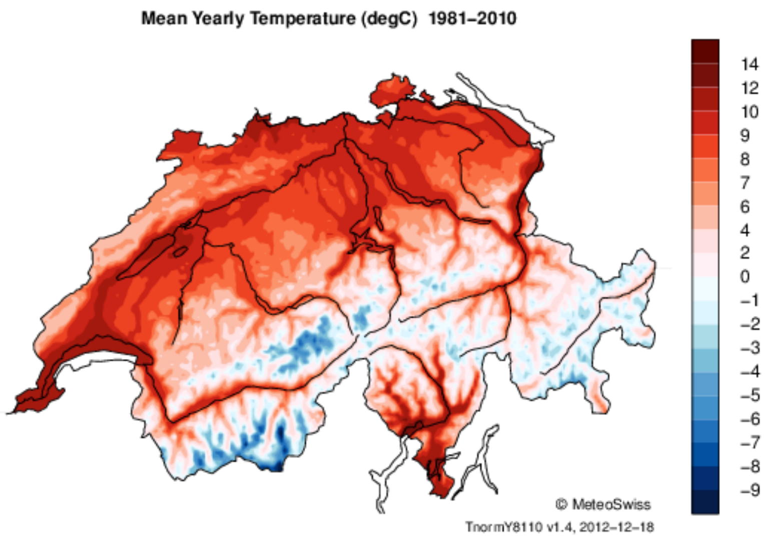

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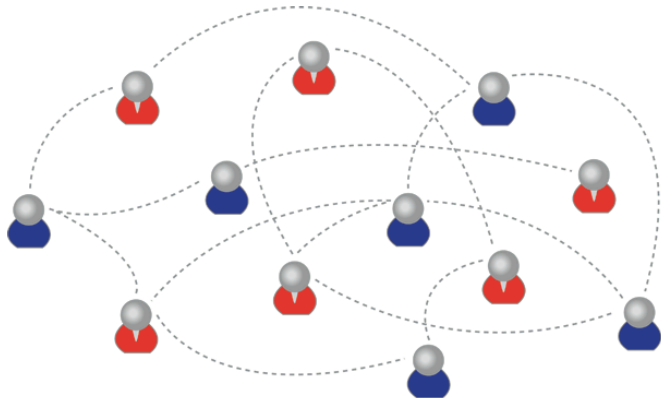


Social network data

We need to take into account the structure behind the data

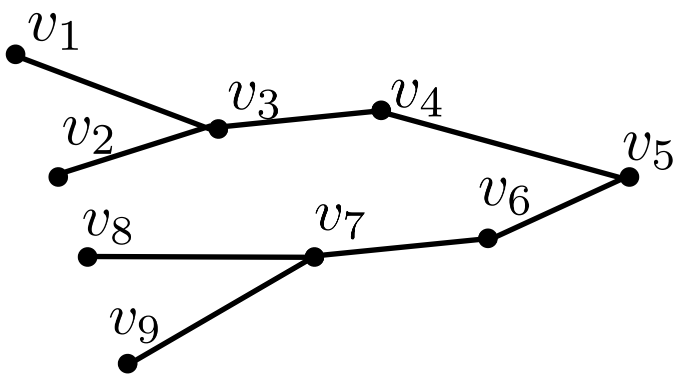
Graphs are appealing tools

- Efficient representations for **pairwise relations** between entities

The Königsberg Bridge Problem
[Leonhard Euler, 1736]

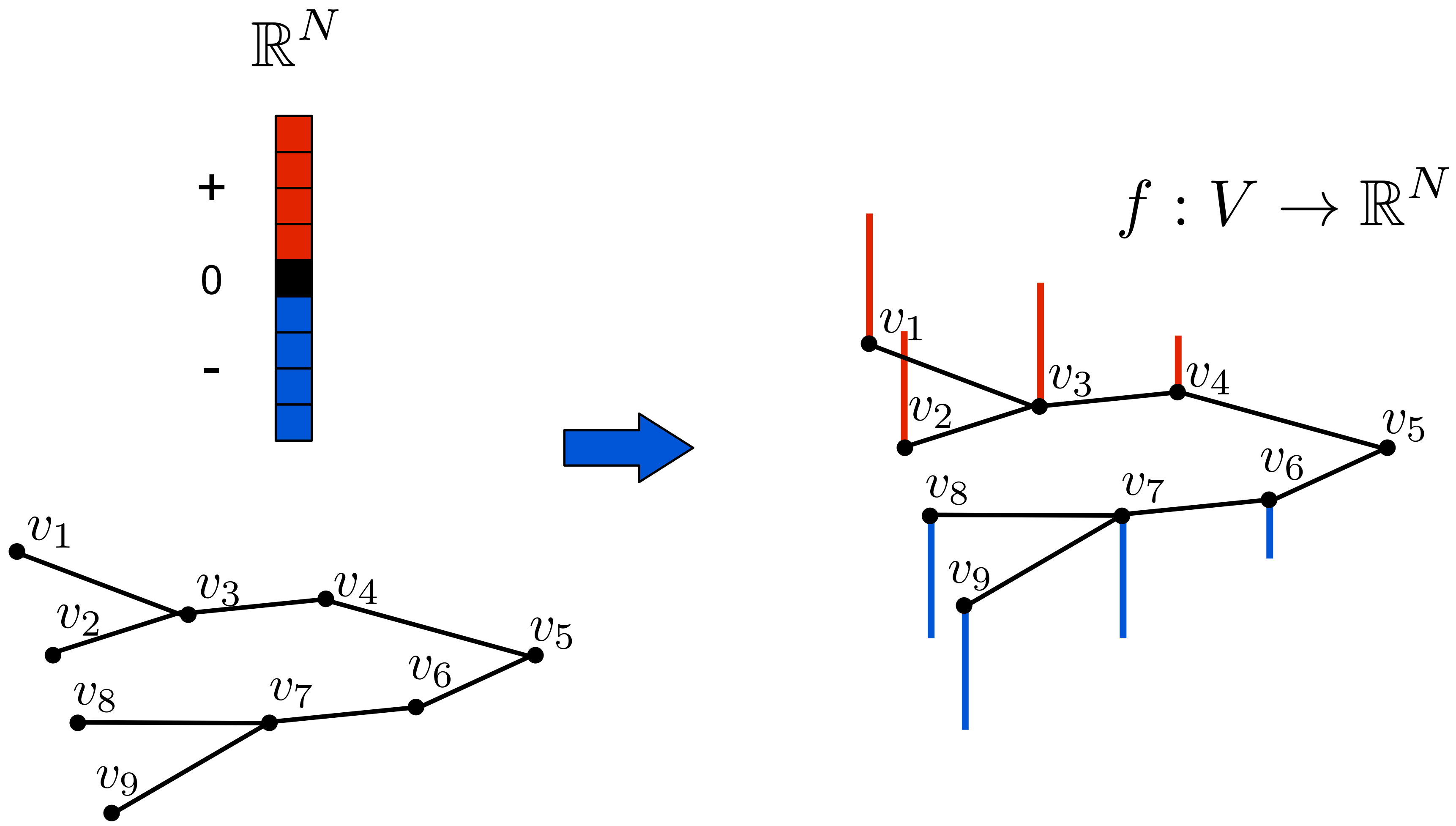
Graphs are appealing tools

- Efficient representations for pairwise relations between entities



Graphs are appealing tools

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



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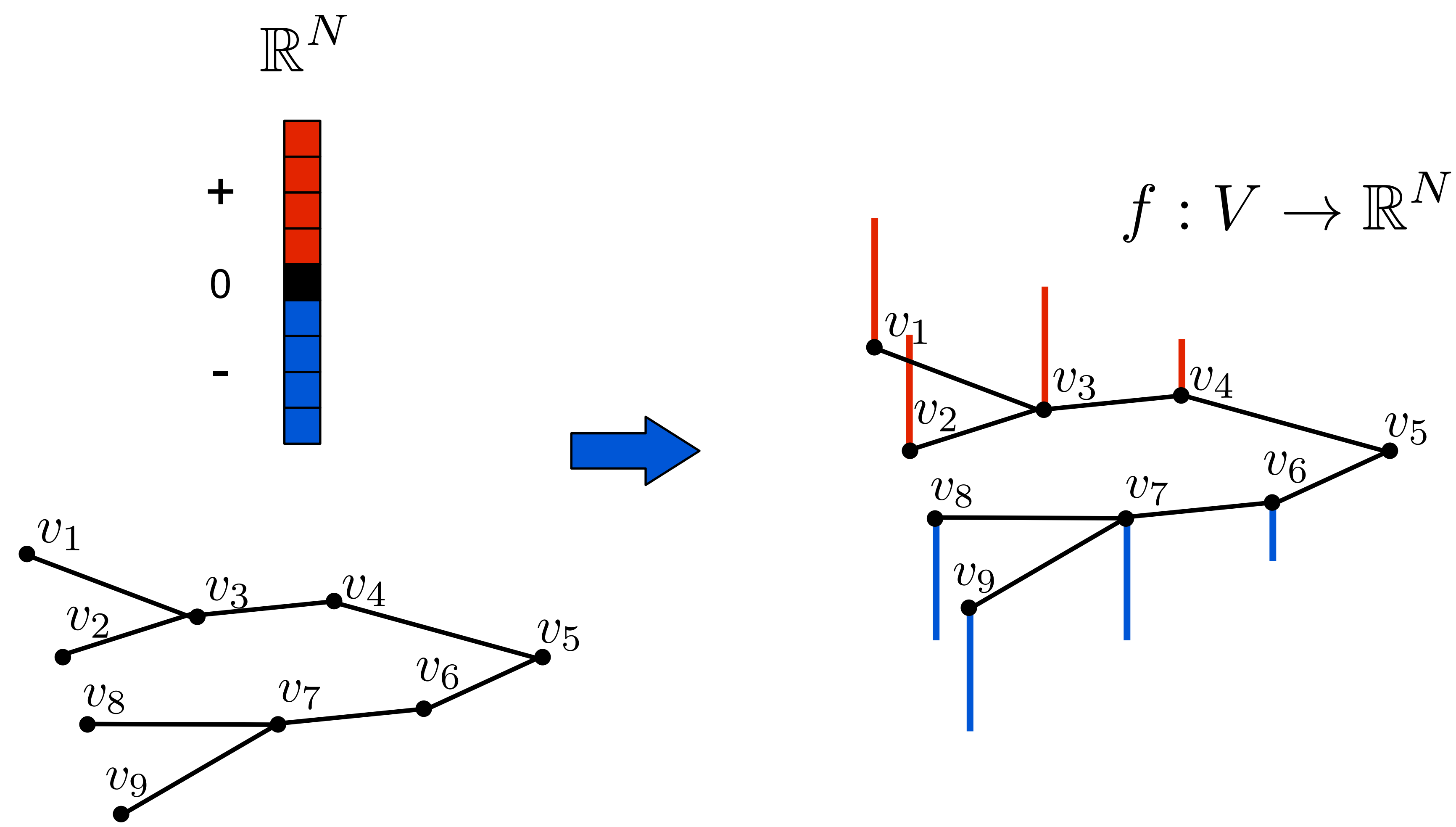
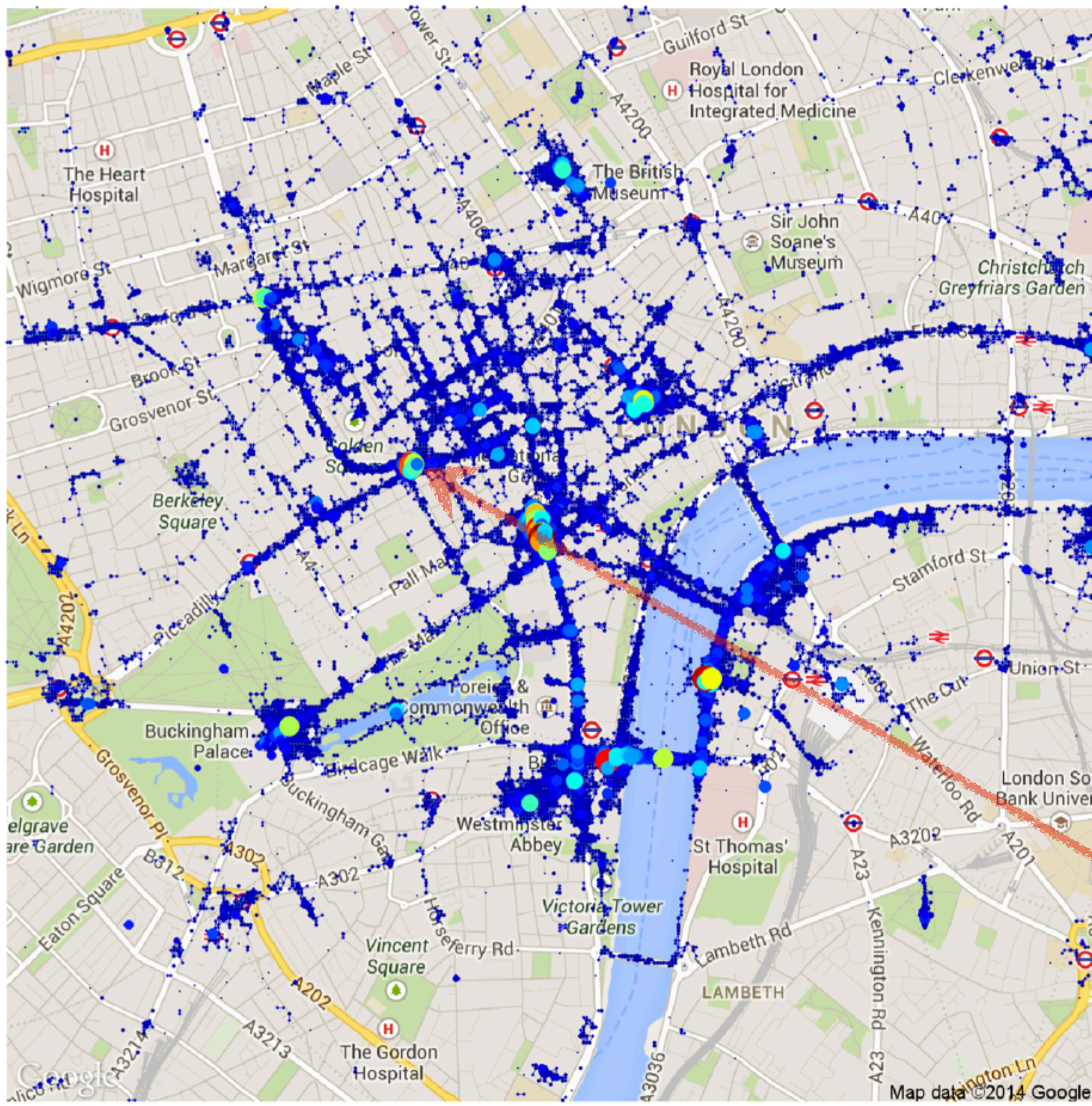
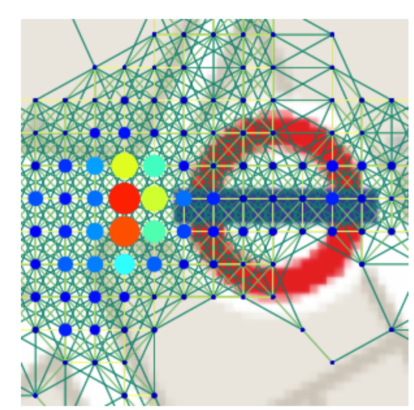


Takes into account both structure (edges) and data (values at vertices)

Graph signals are pervasive



- Vertices:
  - 9000 grid cells in London
- Edges:
  - Connecting cells that are geographically close
- Signal:
  - # Flickr users who have taken photos in two and a half year



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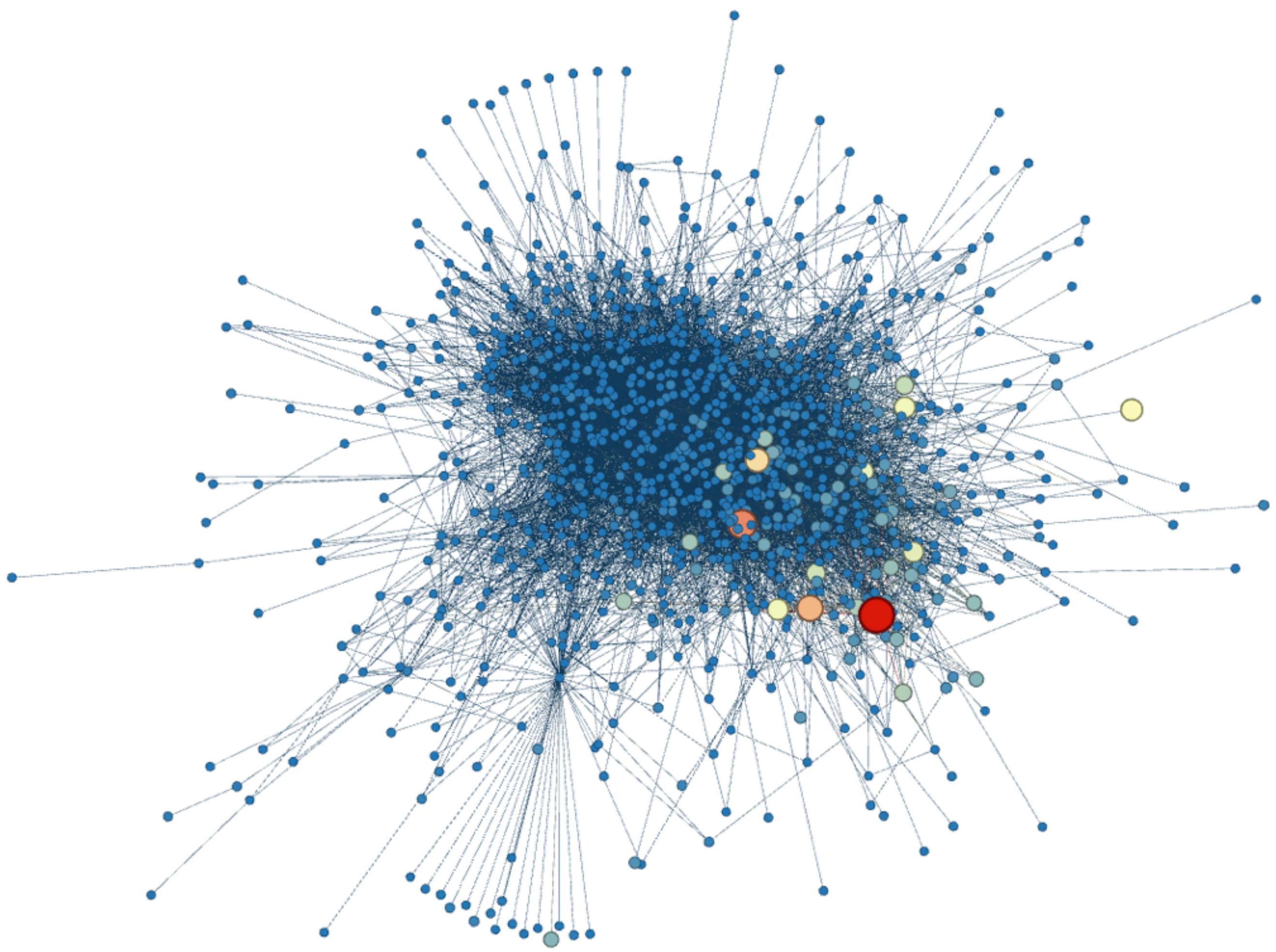
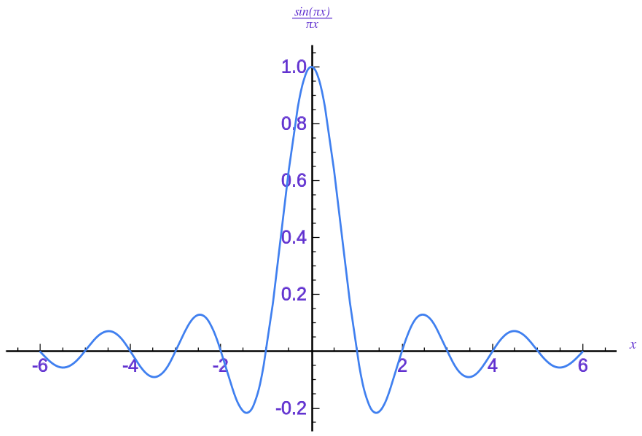
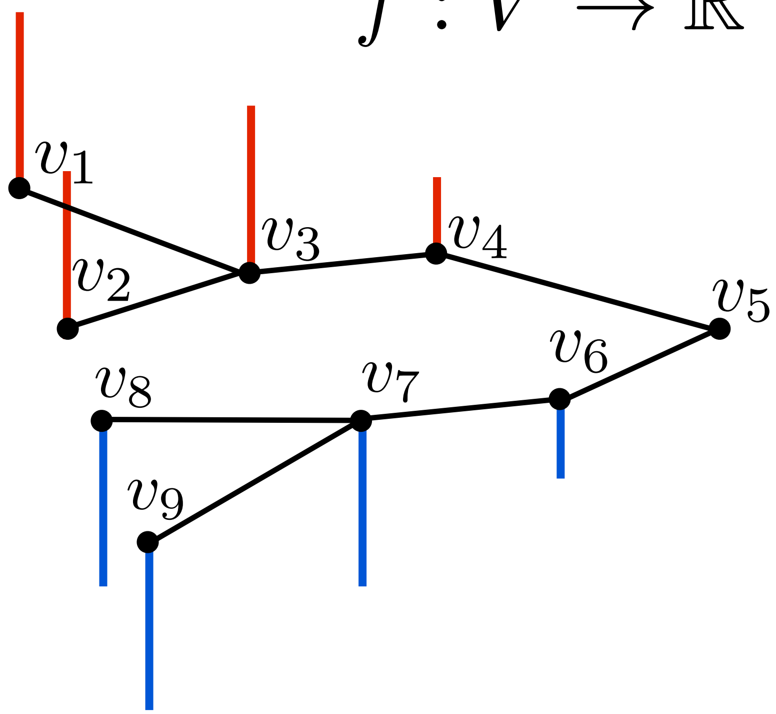


- Vertices:
  - 1000 Twitter users
- Edges:
  - Connecting users that have following relationship
- Signal:
  - # Apple-related hashtags they have posted in six weeks

Research challenges



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



How to generalize 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
- Generalization 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

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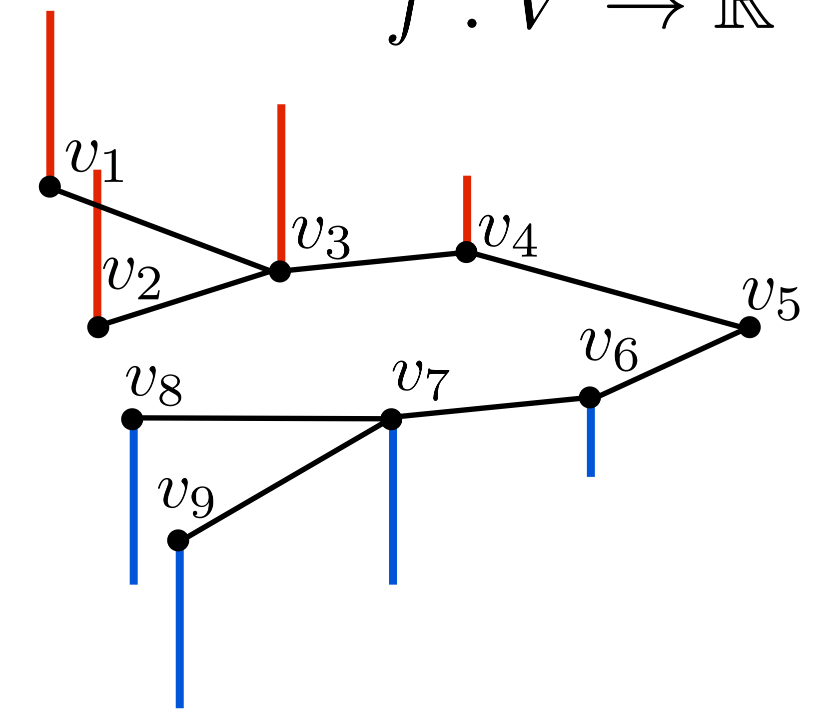

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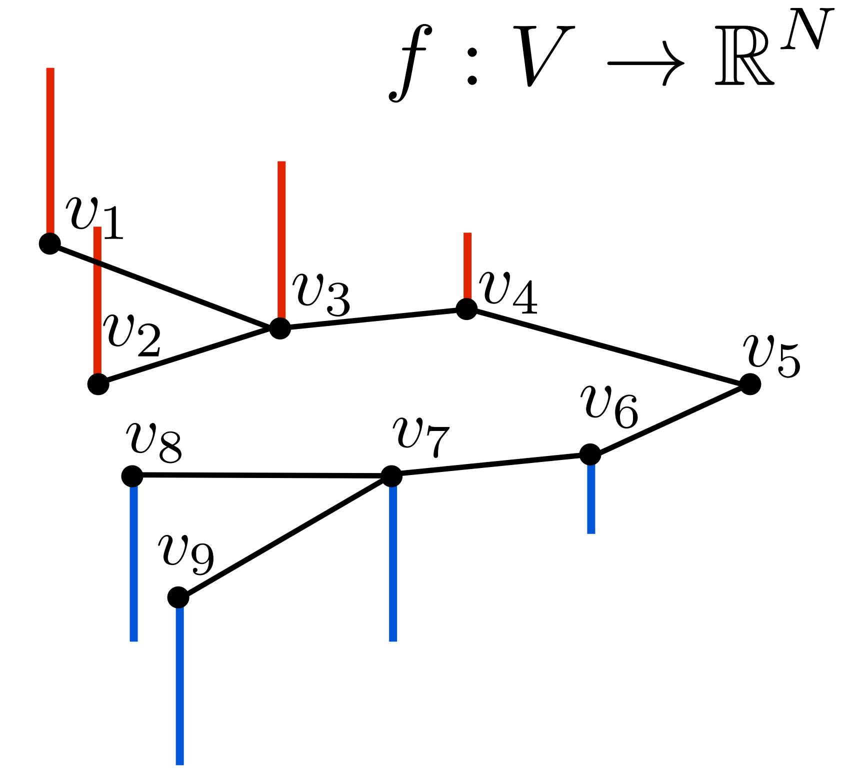
Two paradigms

- The main approaches can be categorized into two families:
  - Vertex (spatial) domain designs
  - Frequency (graph spectral) domain designs



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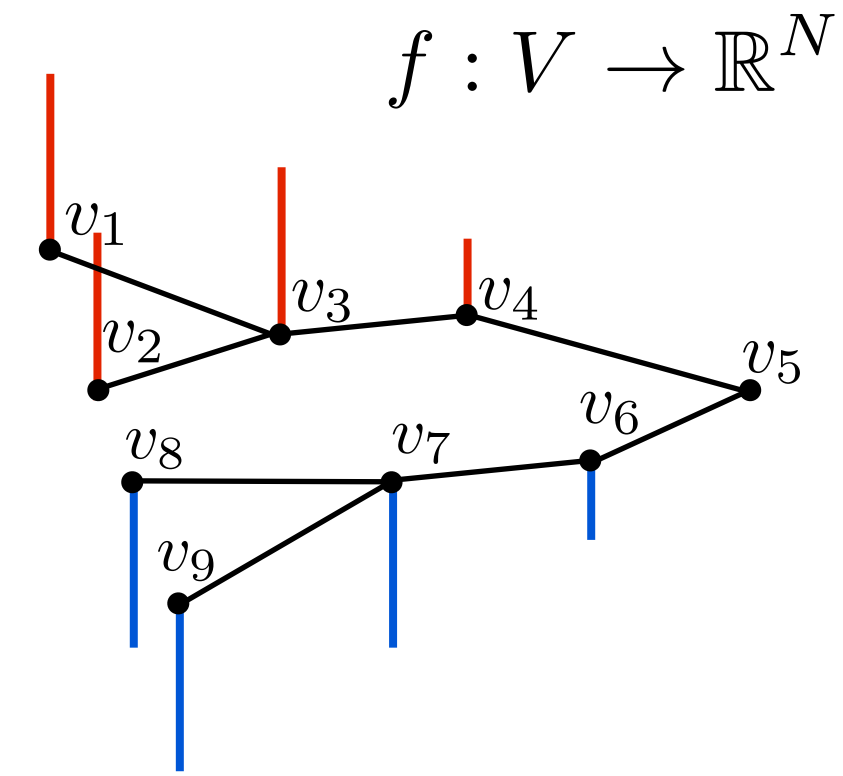
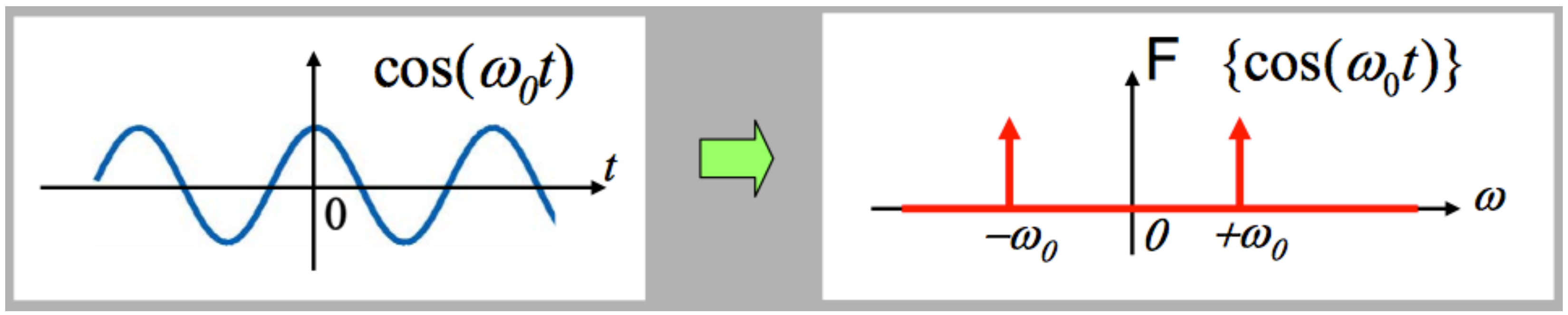
Important for analysis of signal properties

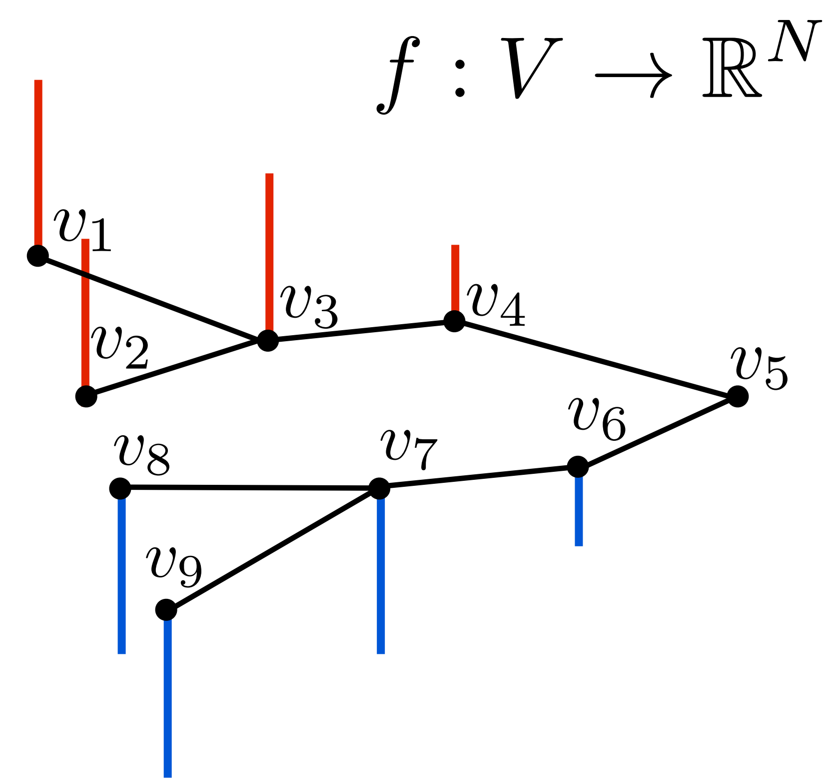


Need for frequency

- Classical Fourier transform provides the frequency domain representation of the signals



Source: http://www.physik.uni-kl.de



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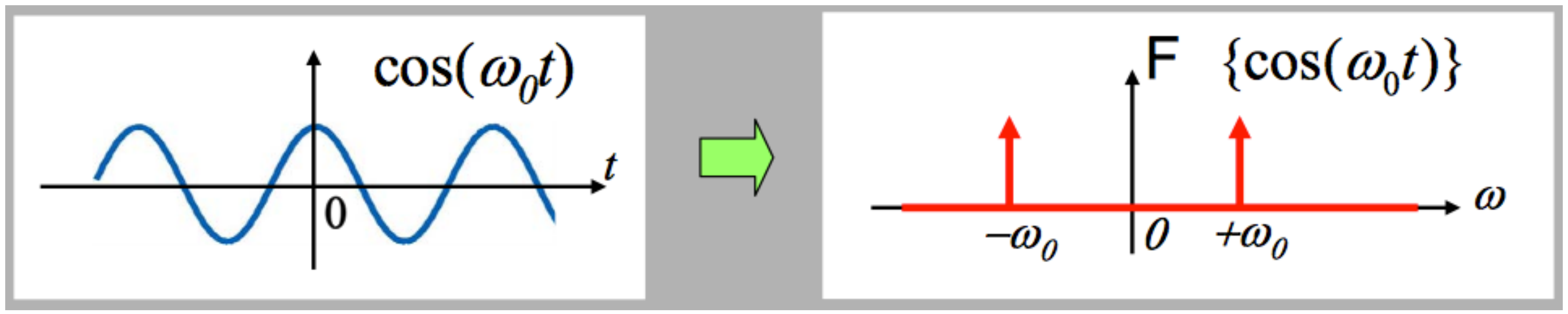

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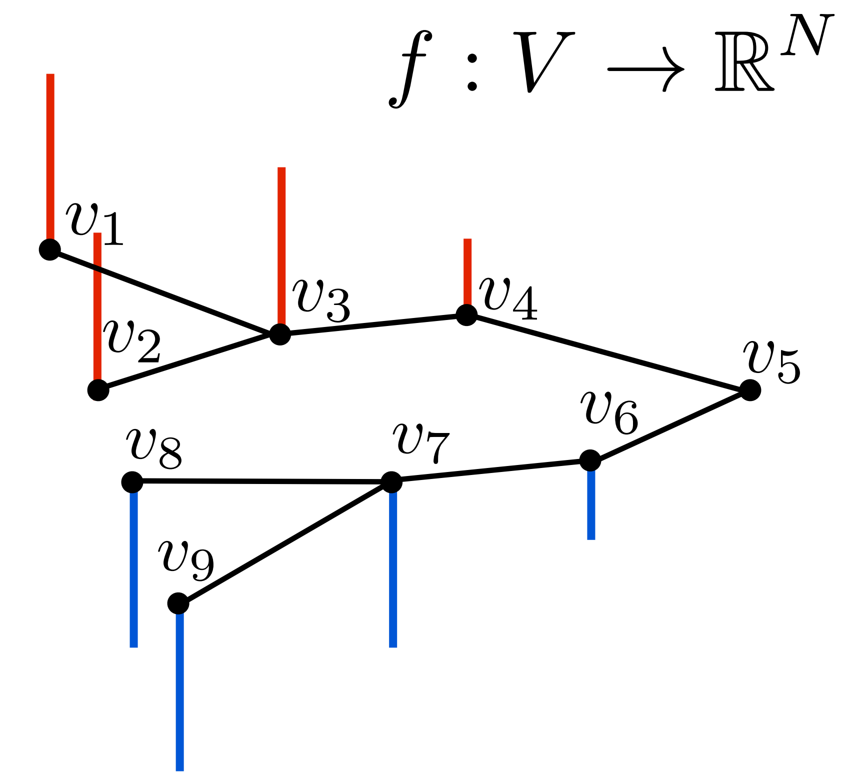
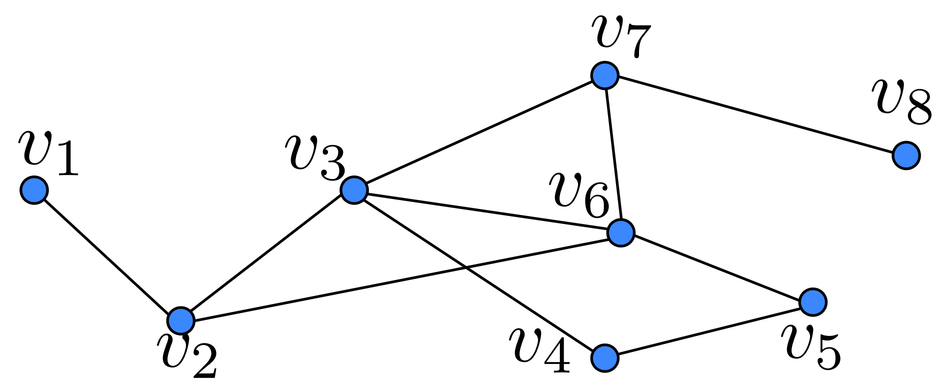
A notion of frequency for graph signals:

We need the graph Laplacian matrix



Graph Laplacian



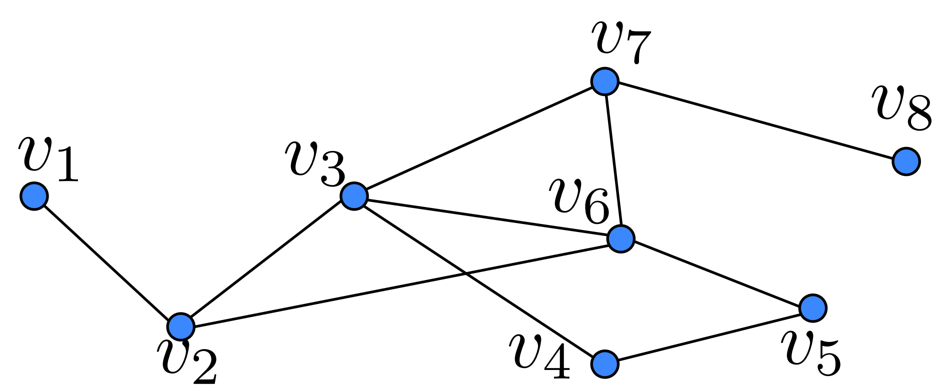
Weighted and undirected graph:

$G = \{V, E\}$

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

A

Graph Laplacian



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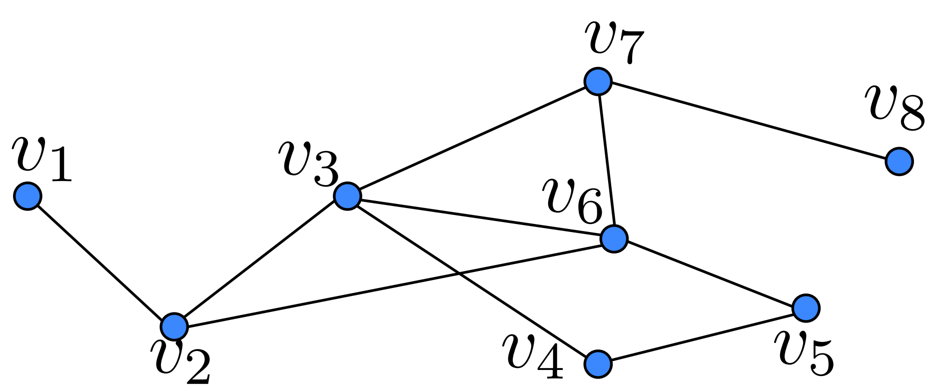
$D = \mathrm{diag}(\mathrm{degree}(v_1) \quad \ldots \quad \mathrm{degree}(v_N))$

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

D $\qquad$ A

Graph Laplacian



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$L = D - A$ **Equivalent to G!**

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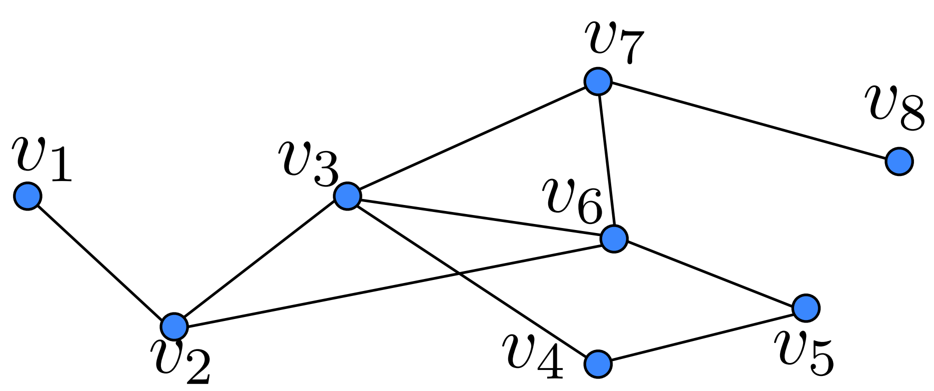
D A L

Graph Laplacian



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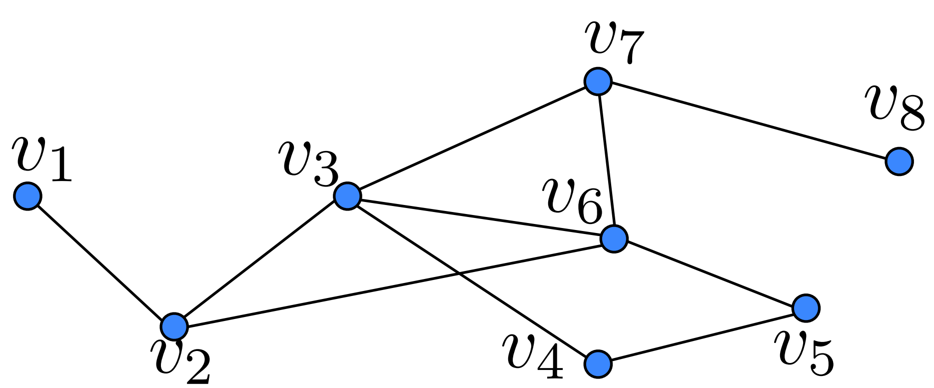
- Symmetric
- Off-diagonal entries non-positive
- Rows sum up to zero

Graph Laplacian



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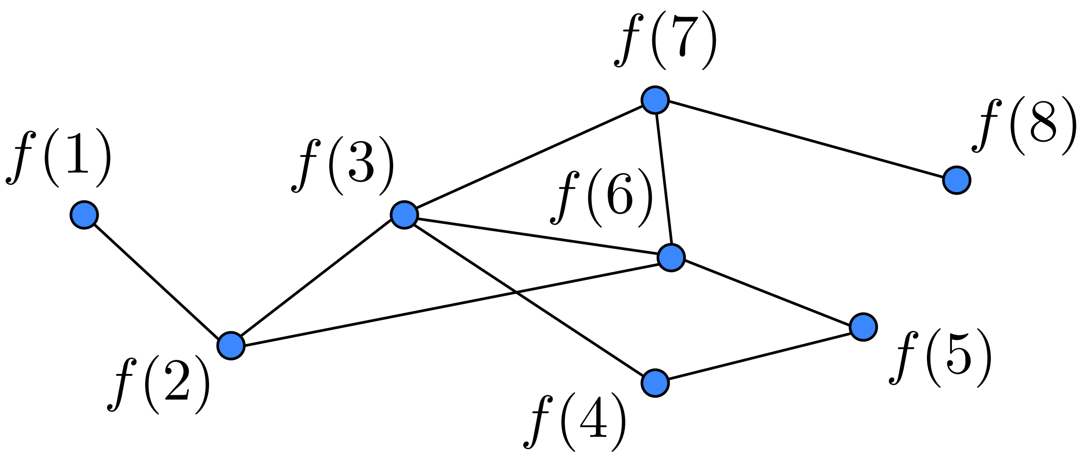
Why graph Laplacian?

- standard stencil approximation of the Laplace operator
- leads to a Fourier-like transform

Graph Laplacian



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

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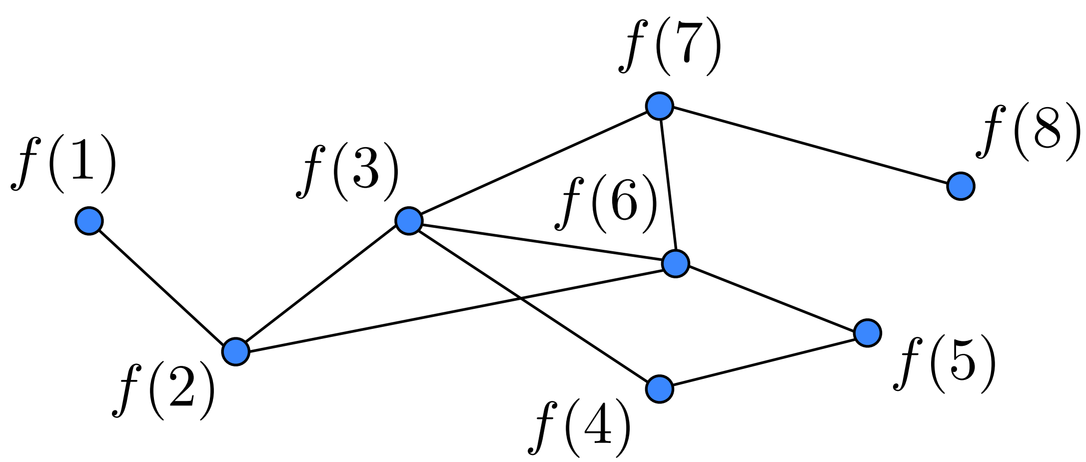
$$L$$

Graph Laplacian



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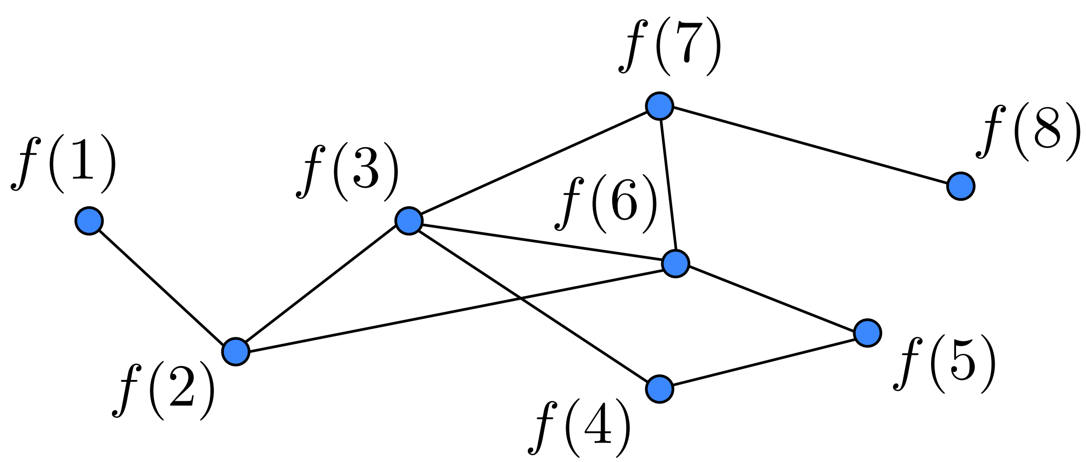
A difference operator:

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

Graph Laplacian



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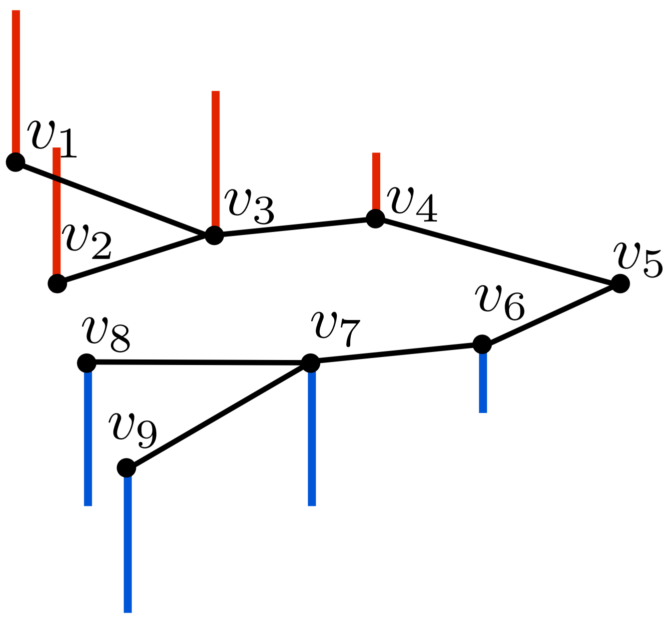
Laplacian quadratic form:

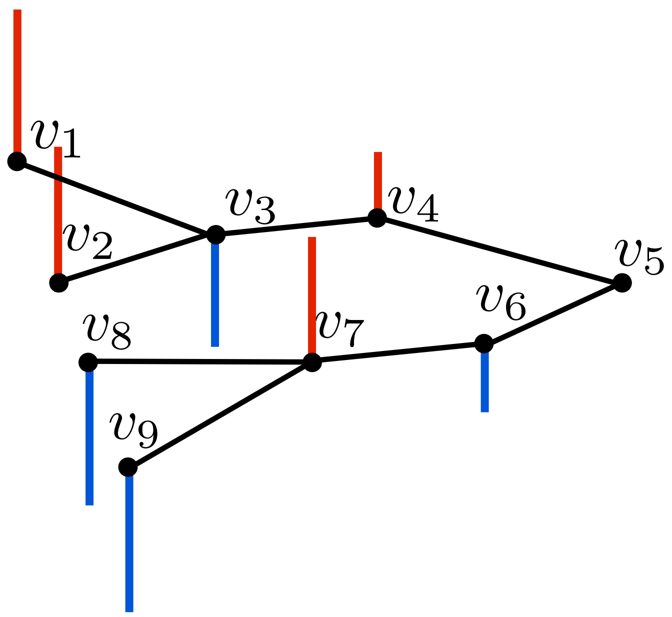
$$f^T L f = \frac{1}{2} \sum_{i,j=1}^{N} A_{ij} \left(f(i) - f(j) \right)^2$$

A measure of "smoothness" [Zhou04]

Graph Laplacian



$f^T L f = 1$



$f^T L f = 21$

Graph Laplacian

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

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

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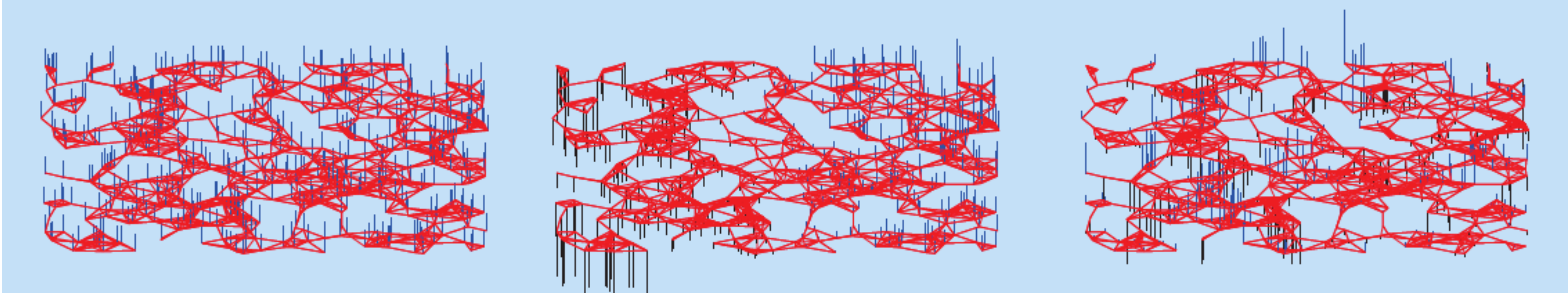
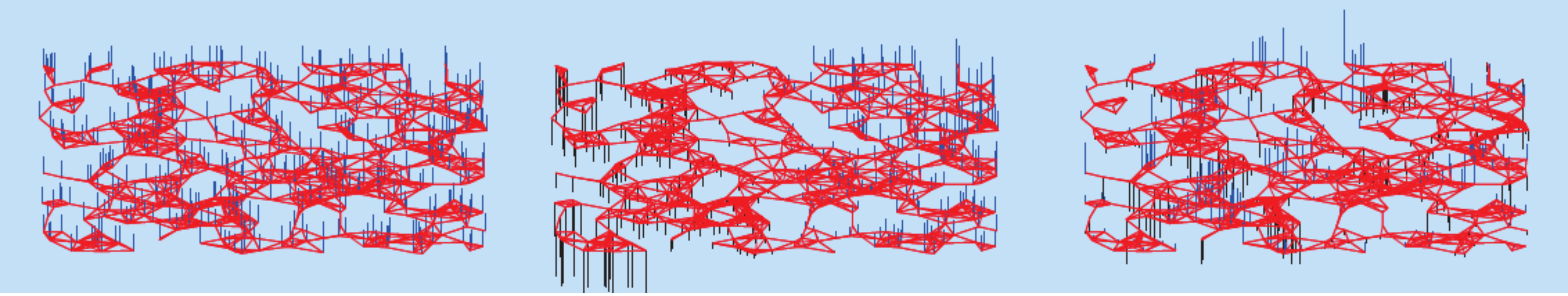
- Eigenvalues are usually sorted increasingly: $0 = \lambda_0 < \lambda_1 \leq \ldots \leq \lambda_{N-1}$

Graph Fourier transform



χ_0 χ_1 χ_{50} [Shuman13]

Graph Fourier transform



χ_0 χ_1 χ_{50} [Shuman13]

Low frequency → High frequency

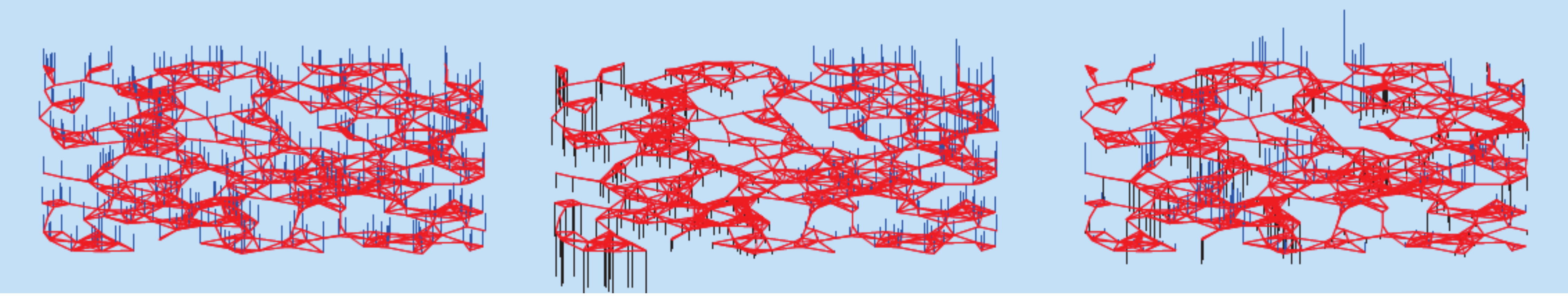
$L = \chi \Lambda \chi^T$

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

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

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

Graph Fourier transform



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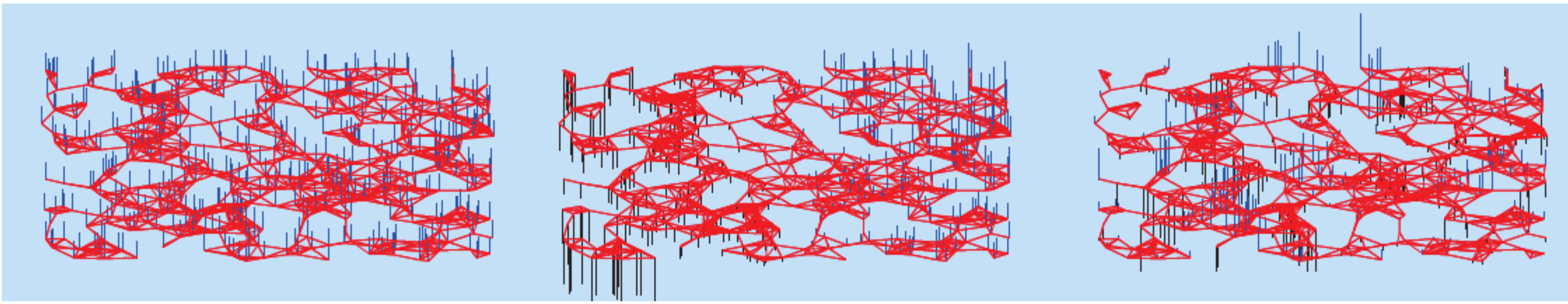
$\chi_{50}^T L \chi_{50} = \lambda_{50}$

Graph Fourier transform:
[Hammond11]

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

Graph Fourier transform



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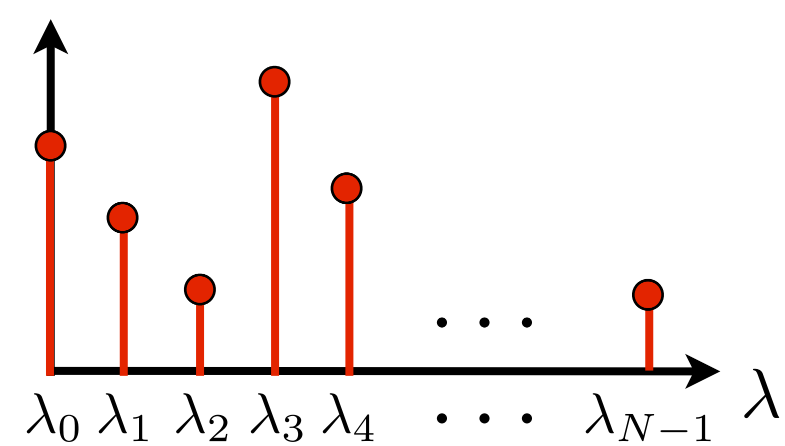
<u>Graph Fourier transform:</u>
[Hammond11]

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



Low frequency High frequency

Graph Fourier transform

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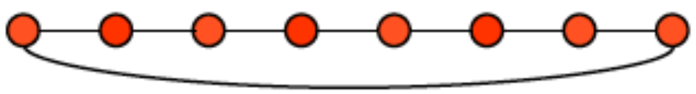
Two special cases



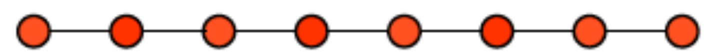
- (Unordered) Laplacian eigenvalues: $\lambda_\ell = 2 - 2\cos\left(\frac{2\ell\pi}{N}\right)$
- One possible choice of orthogonal Laplacian eigenvectors:

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

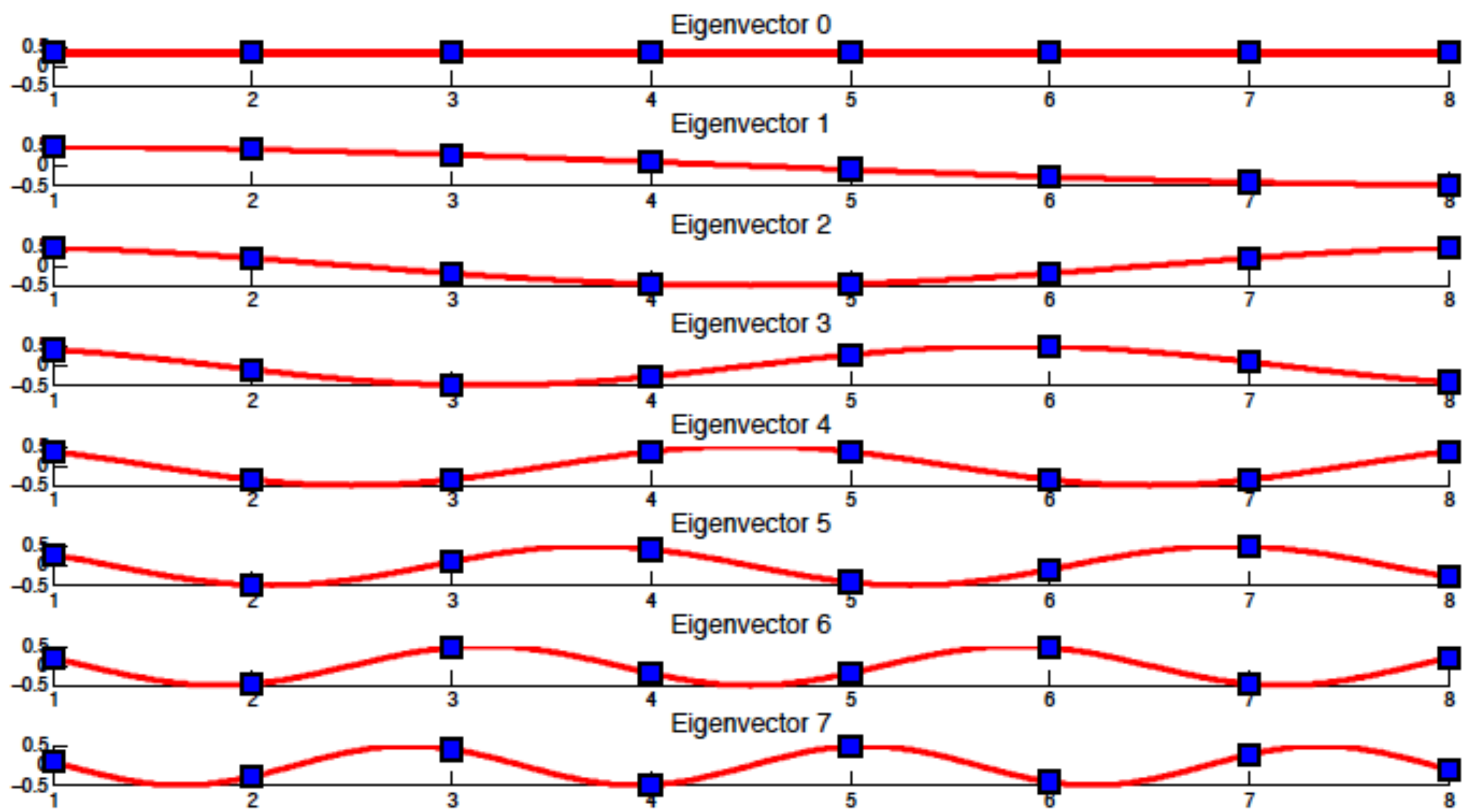
- $\begin{bmatrix} | & & | \\ \chi_0 & \cdots & \chi_{N-1} \\ | & & | \end{bmatrix}$ is the Discrete Fourier Transform (DFT) matrix

[Vandergheynst11]

Two special cases



$\lambda_\ell = 2 - 2\cos\left(\frac{\pi \ell}{N}\right)$ $\chi_0(i) = \frac{1}{\sqrt{N}}$, $\chi_\ell(i) = \sqrt{\frac{2}{N}} \cos\left(\frac{\pi \ell (i-0.5)}{N}\right)$, $\ell = 1, 2, \ldots, N-1$



$\begin{bmatrix} | & & | \\ \chi_0 & \cdots & \chi_{N-1} \\ | & & | \end{bmatrix}$ is the Discrete Cosine Transform matrix (DCT-II, Strang, 1999), which is used in JPEG image compression

[Vandergheynst11]

Outline

- Motivation
- Graph signal processing (GSP): Basic concepts
- Spectral filtering: Basic tools of GSP
- Applications and perspectives

Classical frequency filtering

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

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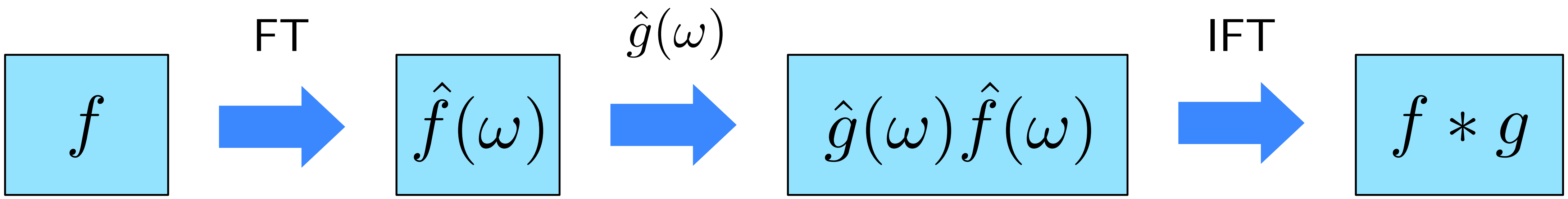
Apply filter with transfer function $\hat{g}(\cdot)$ to a signal f



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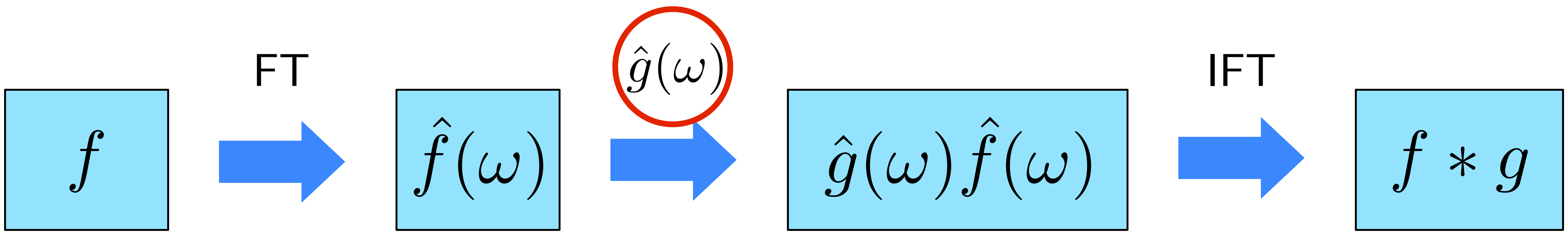

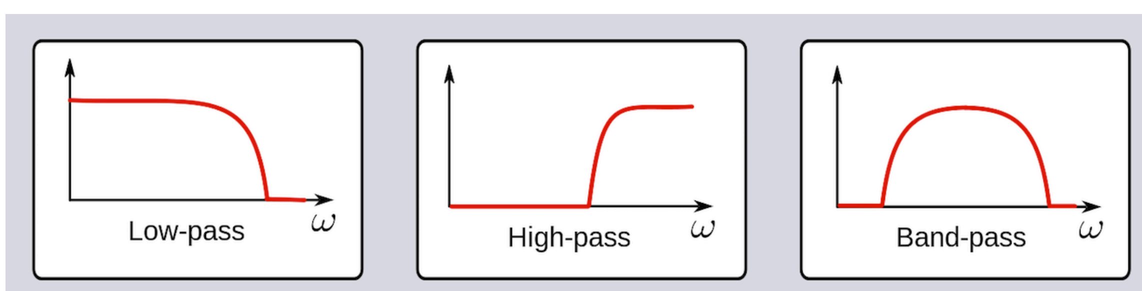

Graph spectral filtering

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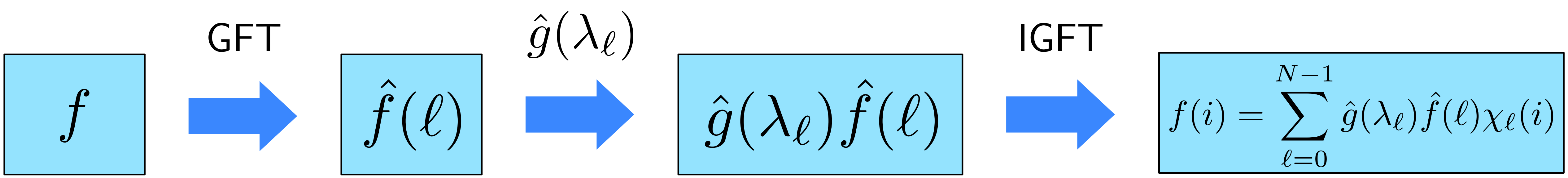

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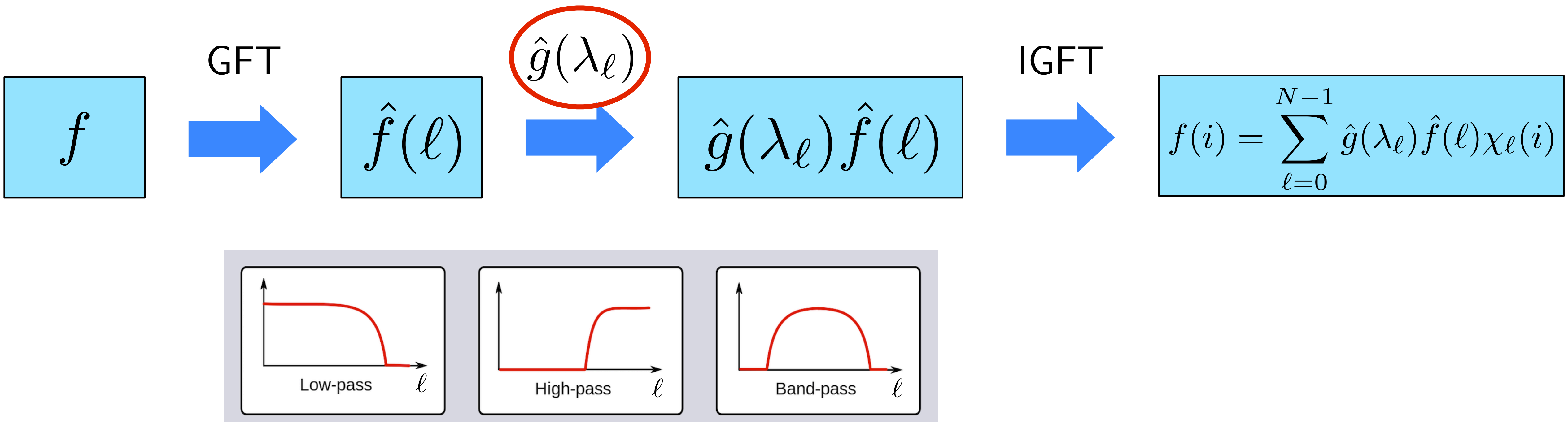

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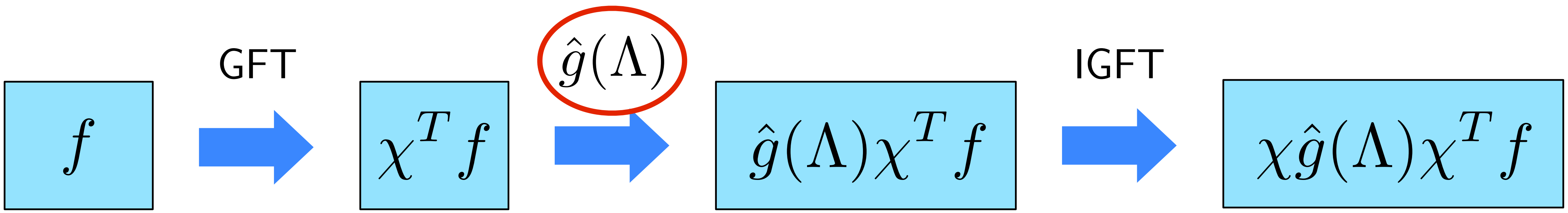

$$\hat{g}(\Lambda) = \begin{bmatrix} \hat{g}(\lambda_0) & & 0 \\ & \ddots & \\ 0 & & \hat{g}(\lambda_{N-1}) \end{bmatrix}$$

Graph Laplacian revisited

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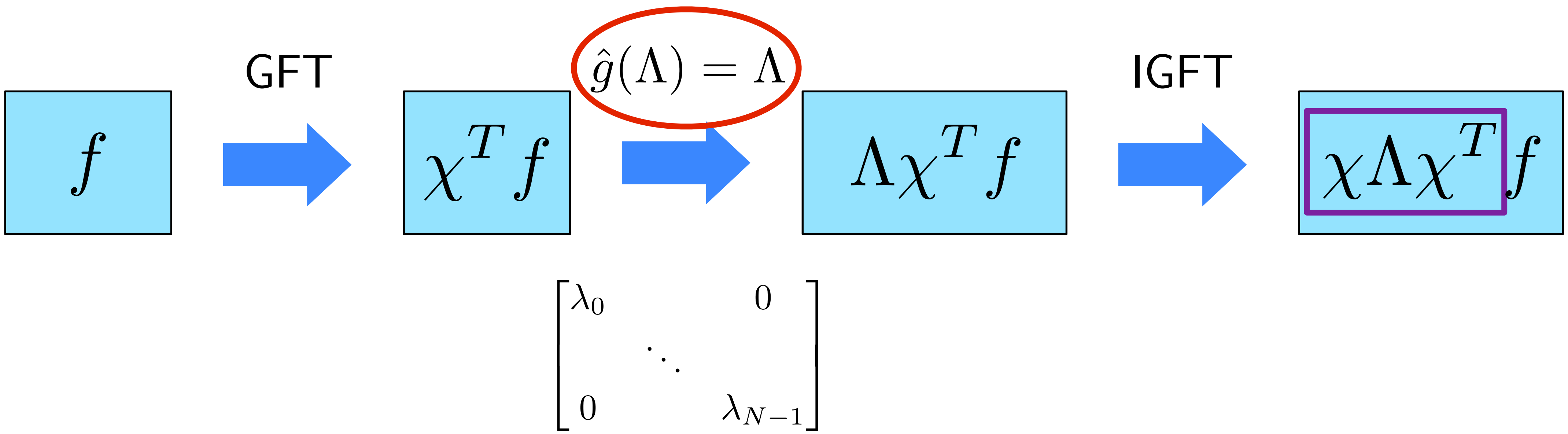
The Laplacian L is a difference operator: $Lf = \chi \Lambda \chi^T f$



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

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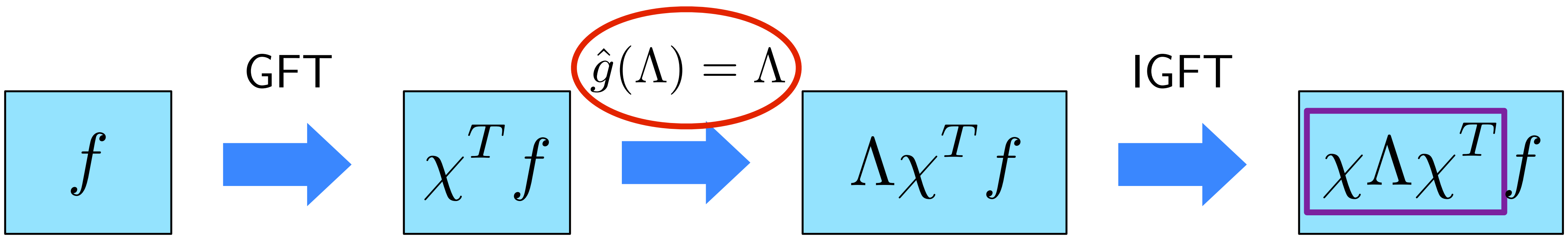

$$\begin{bmatrix} \lambda_0 & & 0 \\ & \ddots & \\ 0 & & \lambda_{N-1} \end{bmatrix}$$

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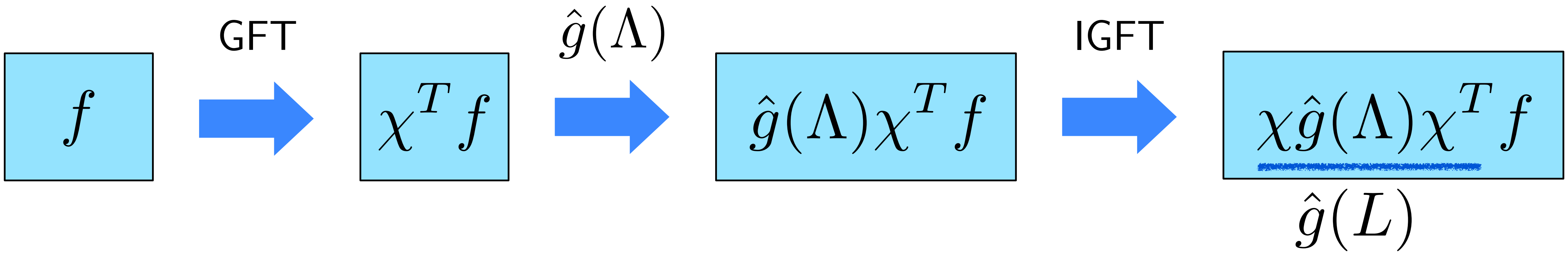
The Laplacian quadratic form: $f^T L f = ||L^{\frac{1}{2}} f||_2 = ||\chi \Lambda^{\frac{1}{2}} \chi^T f||_2$

Graph transform/dictionary design

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



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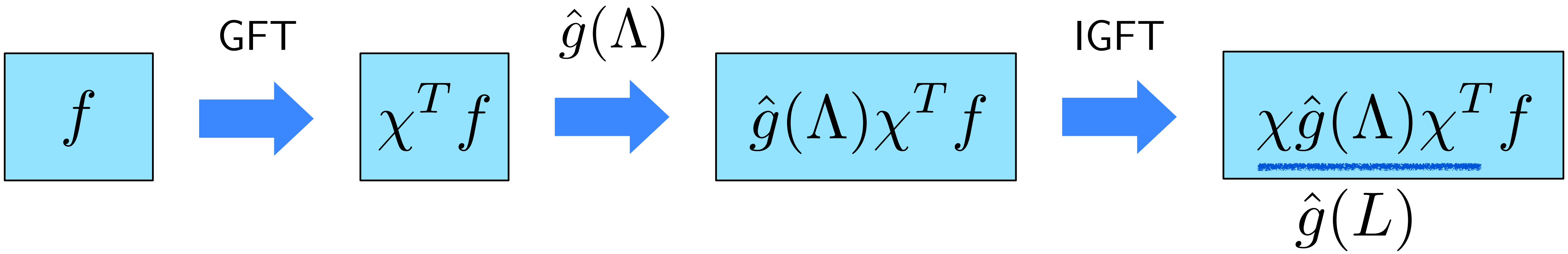
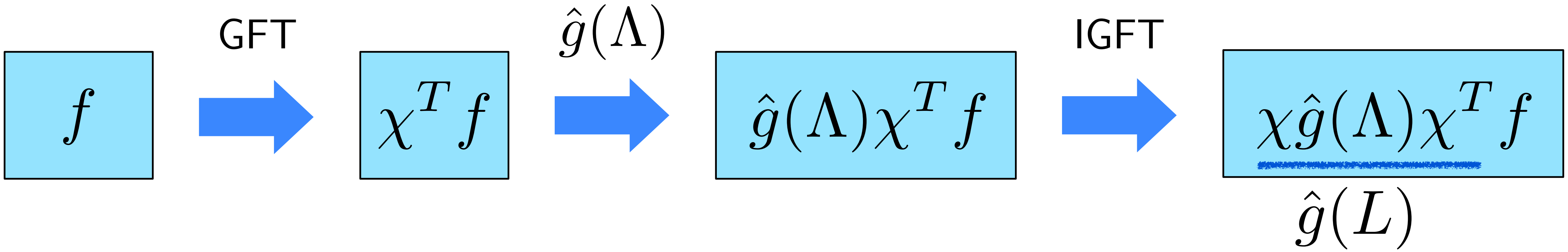


- Important properties can be achieved by properly defining $\hat{g}(L)$, such as localization of atoms

- Closely related to kernels and regularization on graphs [Smola03]

A simple example



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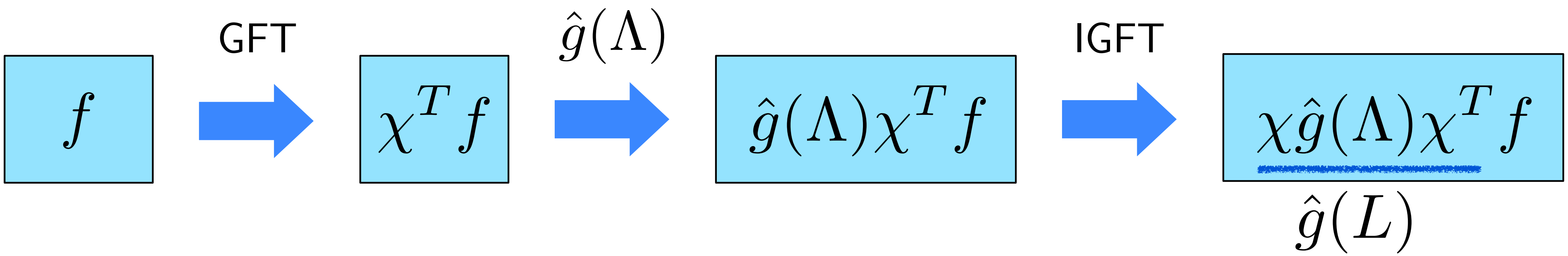

Problem: We observe a noisy graph signal $f = y_0 + \eta$ and wish to recover y_0

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

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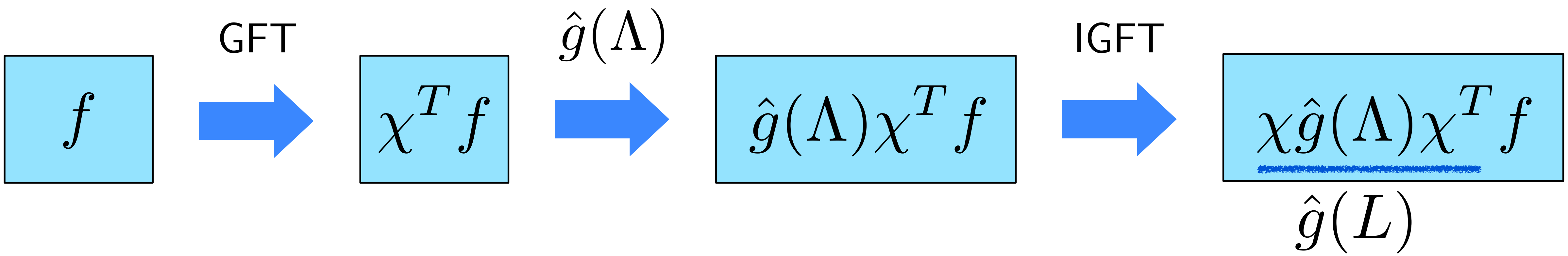

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Data fitting term

"Smoothness" assumption

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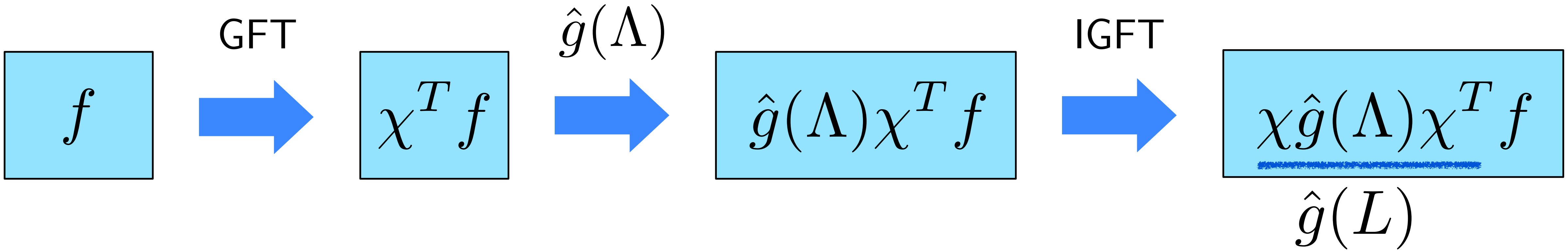

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Data fitting term

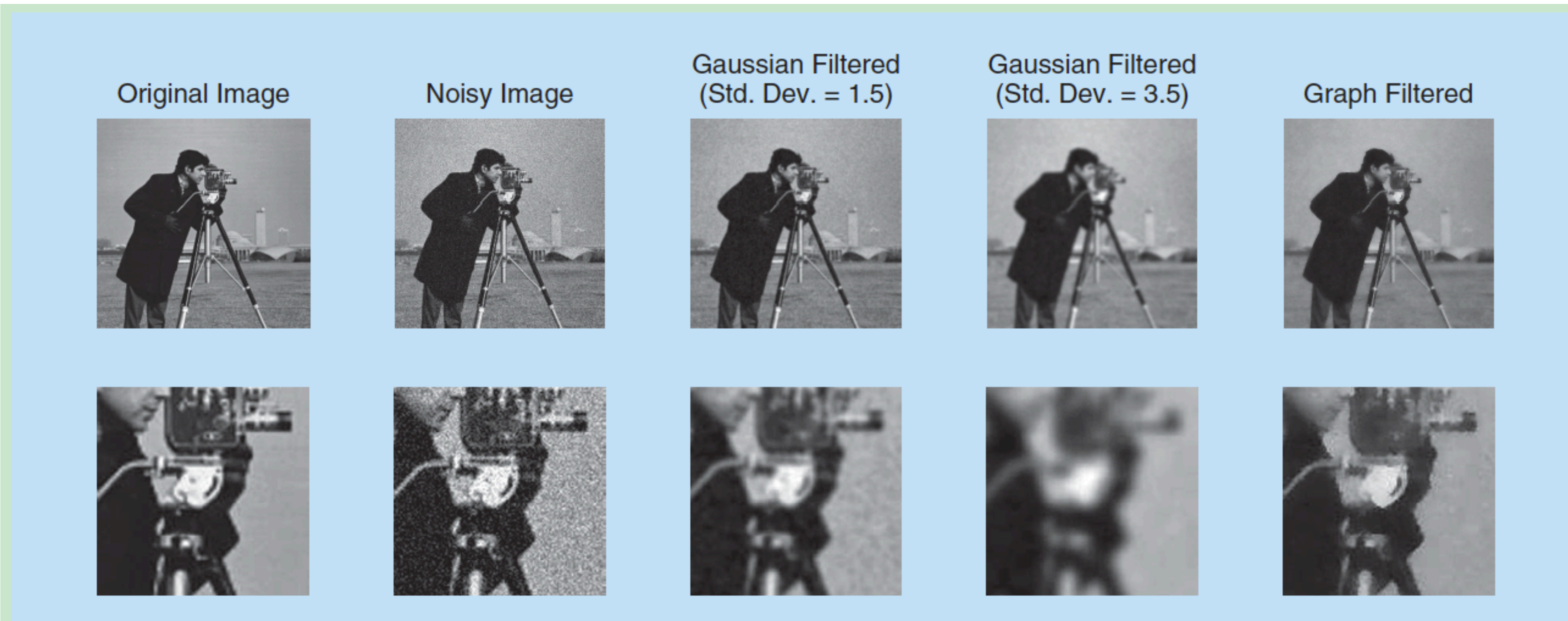
"Smoothness" assumption

$$y^* = \underbrace{(I + \gamma L)^{-1}}_{\hat{g}(L)} f$$

Laplacian (Tikhonov) regularization is equivalent to low-pass filtering in the graph spectral domain!

Example designs

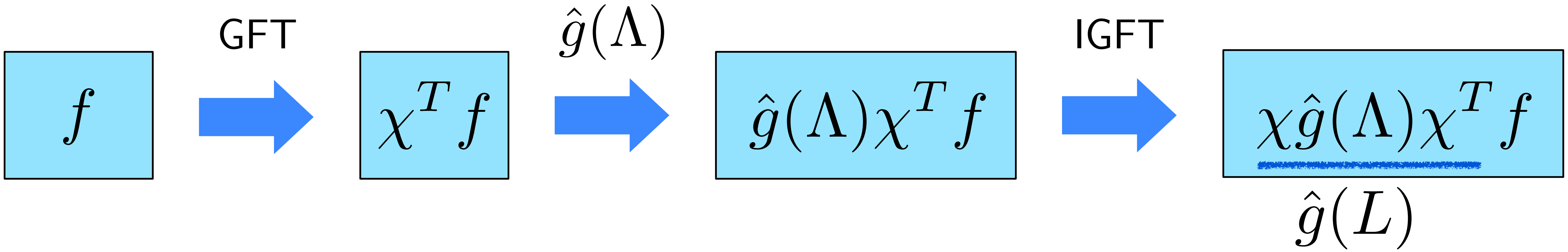
- Consider a noisy image as the observed noisy graph signal
- Consider a regular grid graph (weights inv. prop. to pixel value difference)



[FIGS2] Image denoising via classical Gaussian filtering and graph spectral filtering.

[Shuman13]

Example designs



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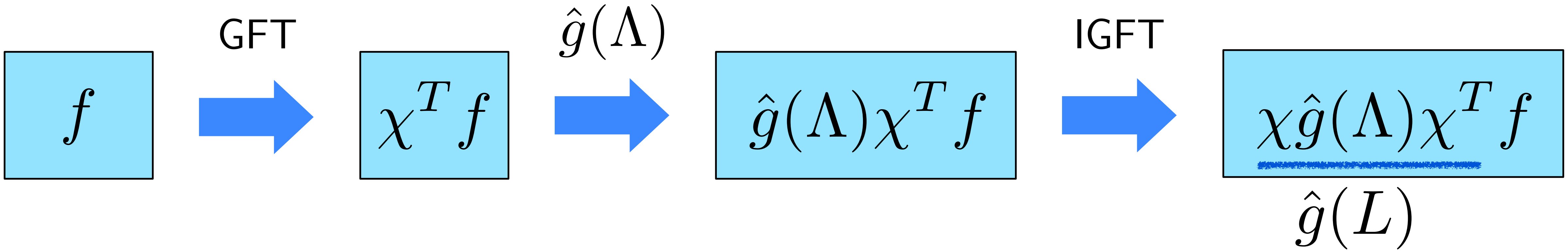

Low-pass filters: $\hat{g}(L) = (I + \gamma L)^{-1} = \chi(I + \gamma\Lambda)^{-1}\chi^T$

Shifted and dilated band-pass filters: Spectral graph wavelets $\hat{g}(sL)$ [Hammond11, Shuman11, Dong13]

Window kernel: Windowed graph Fourier transform [Shuman12]

Parametric polynomials: $\hat{g}_s(L) = \sum_{k=0}^{K} \alpha_{sk} L^k = \chi(\sum_{k=0}^{K} \alpha_{sk} \Lambda^k)\chi^T$ [Thanou14]

Adapted kernels: Learn values of $\hat{g}(L)$ directly from data [Zhang12]

Spectral graph wavelets

$$\psi_{s,a}(x) = \frac{1}{s}\psi\left(\frac{x-a}{s}\right)$$

$$W_f(s,a) = \int_{-\infty}^{\infty} \frac{1}{s}\psi^*\left(\frac{x-a}{s}\right) f(x)\,dx$$

$$\bar{\psi}_s(x) = \frac{1}{s}\psi^*\left(\frac{-x}{s}\right)$$

$$(T^s f)(a) = \int_{-\infty}^{\infty} \frac{1}{s}\psi^*\left(\frac{x-a}{s}\right) f(x)\,dx = \int_{-\infty}^{\infty} \bar{\psi}_s(a-x) f(x)\,dx$$

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Fourier multiplier operator: scaled kernel $\hat{\psi}^*(s\omega)$

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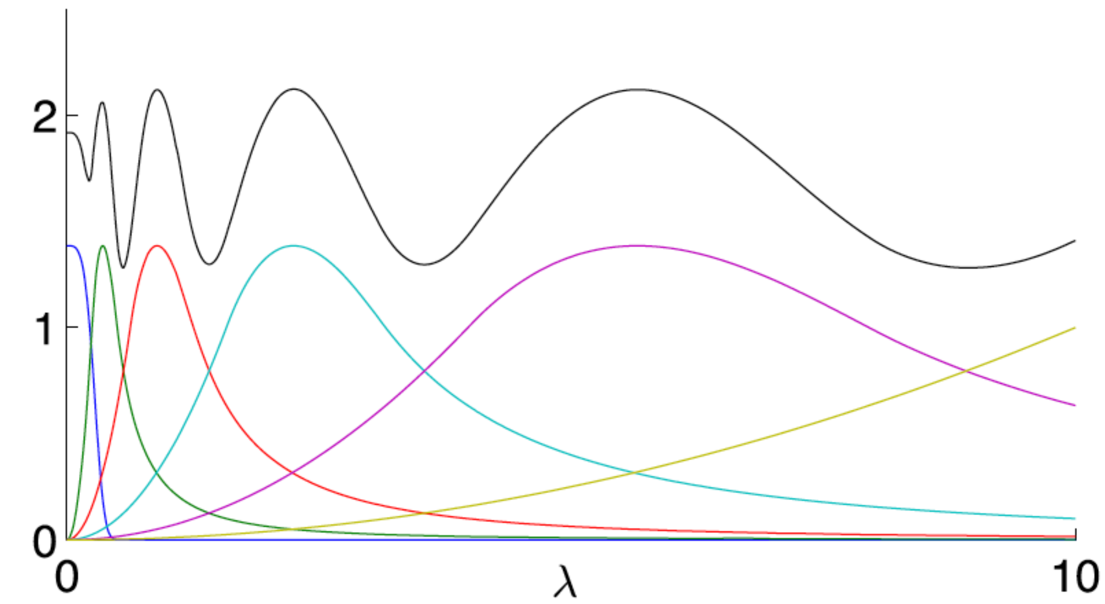

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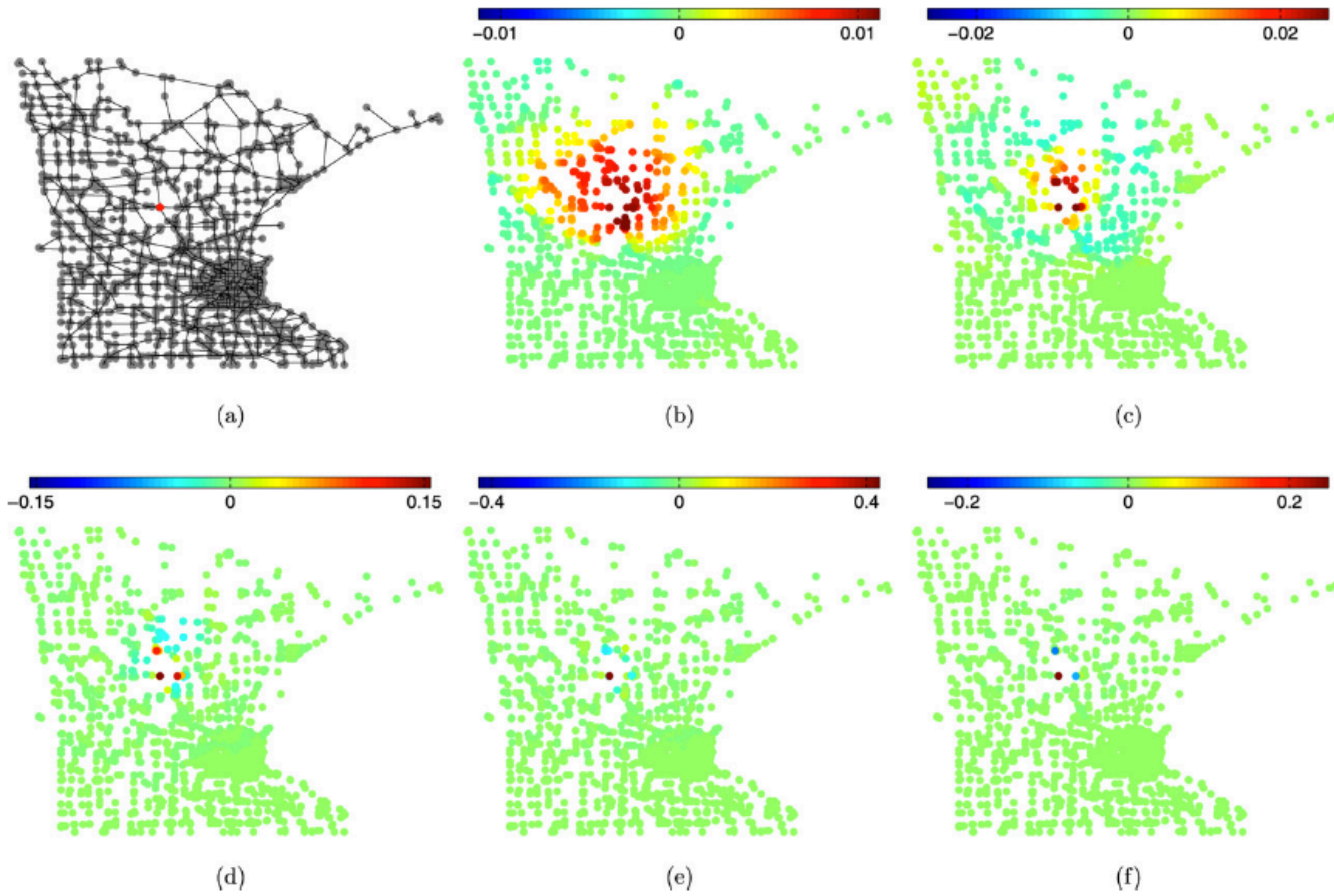

Fig. 4. Spectral graph wavelets on Minnesota road graph, with $K = 100$, $J = 4$ scales. (a) Vertex at which wavelets are centered, (b) scaling function, (c)–(f) wavelets, scales 1–4.

[Hammond11]

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Applications of GSP

- Signal processing and machine learning tasks
  - Denoising [Graichen15, Liu16]
  - Semi-supervised learning / Classification [Kipf16, Manessi17]
  - Clustering [Tremblay14, Tremblay16]
  - Dimensionality reduction [Rui16]

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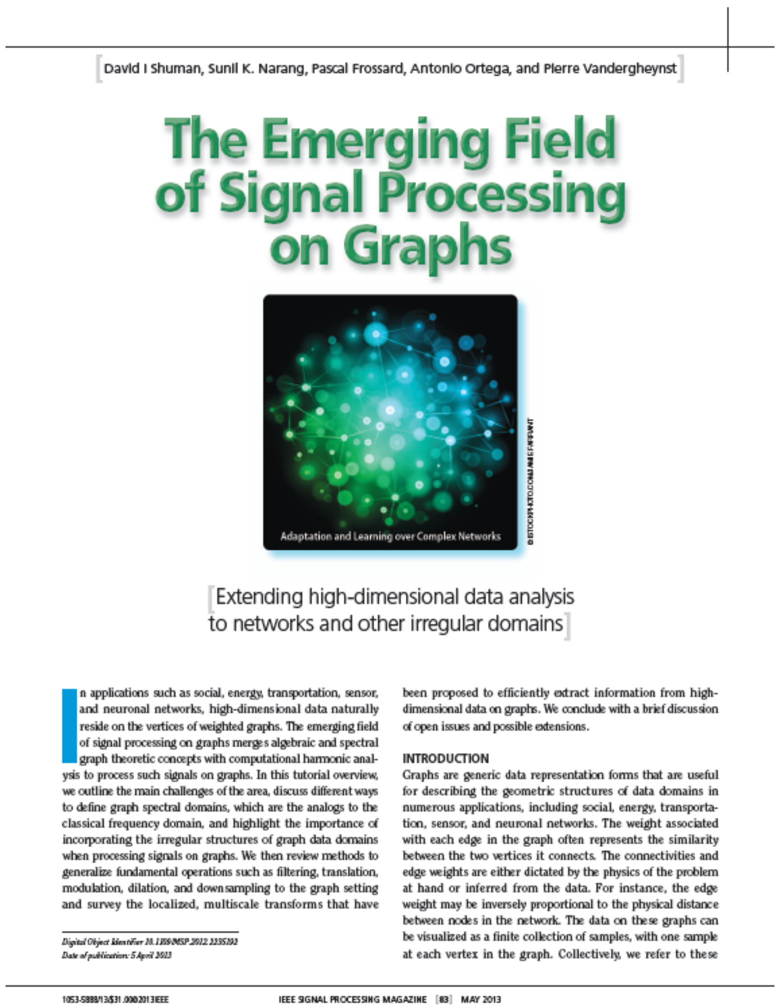
  - Clustering [Tremblay14, Tremblay16]
  - Dimensionality reduction [Rui16]
- Application domains
  - Neuroimaging / Brain activity analysis [Huang16, Smith17, Ktena17]
  - Social network analysis (e.g., community detection [Bruna17], recommendation [Monti17], link prediction [Schlichtkrull17])
  - Urban computing (e.g., mobility inference [Dong13])
  - Computer graphics [Monti16, Yi16, Wang17, Simonovsky17]
  - Geoscience and remote sensing [Bayram17]

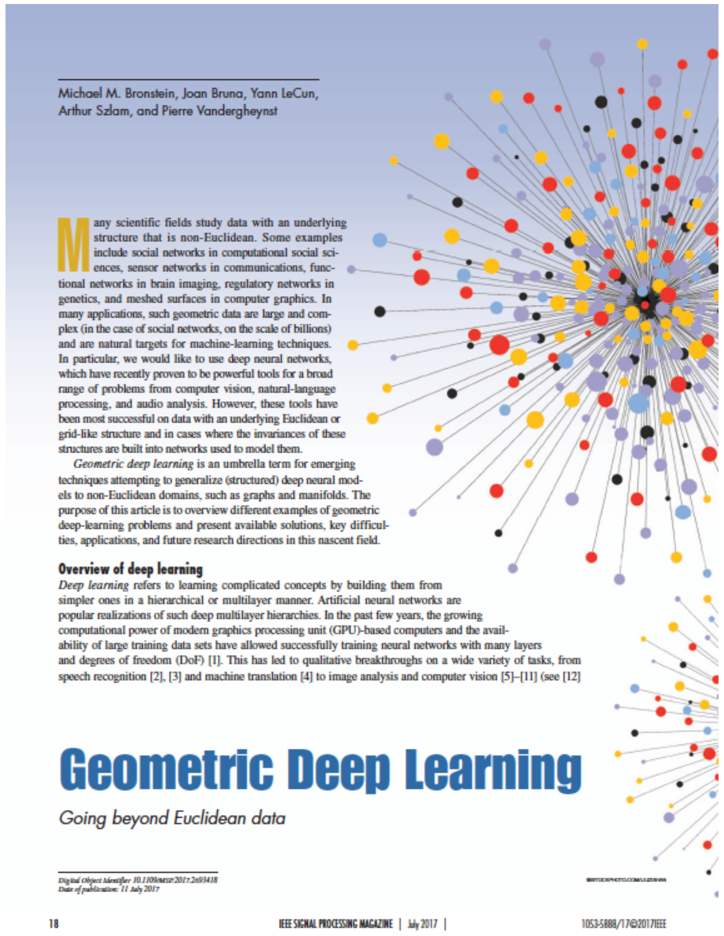
Future of GSP

- 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)
- Applications

References

- Three review papers:





Resources

- Graph signal processing
  - MATLAB toolbox: https://lts2.epfl.ch/gsp/
  - Python toolbox: https://pygsp.readthedocs.io/en/stable/
- Spectral graph wavelet transform
  - MATLAB toolbox: https://wiki.epfl.ch/sgwt
  - Python toolbox: https://github.com/aweinstein/pysgwt
- Topology inference
  - Tutorial: http://web.media.mit.edu/~xdong/presentation/GSP_GraphLearning.pdf
- Geometric deep learning
  - Workshops, tutorials, papers and code: http://geometricdeeplearning.com

contact: xiaowen.dong@eng.ox.ac.uk