

Graph Signal Processing for Machine Learning

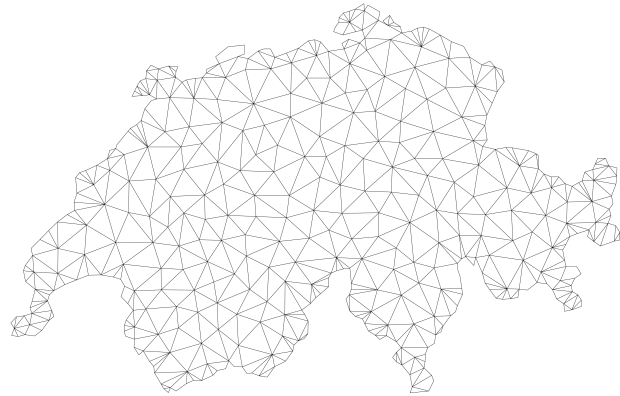
A Review and New Perspectives

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Michael Bronstein, Pascal Frossard

ICASSP Tutorial, June 2021



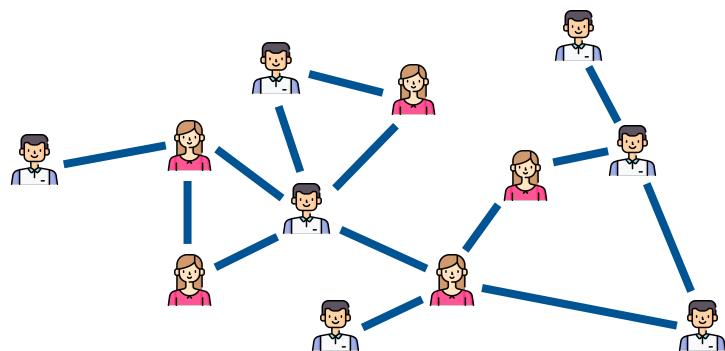
Networks are pervasive



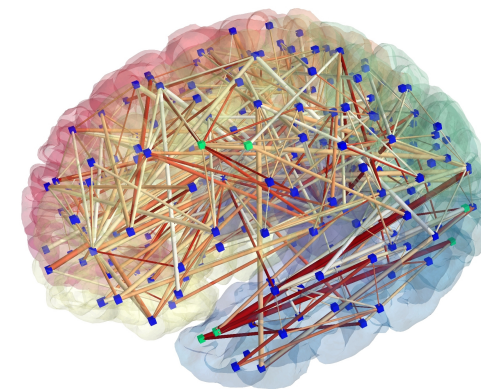
geographical network



traffic network



social network

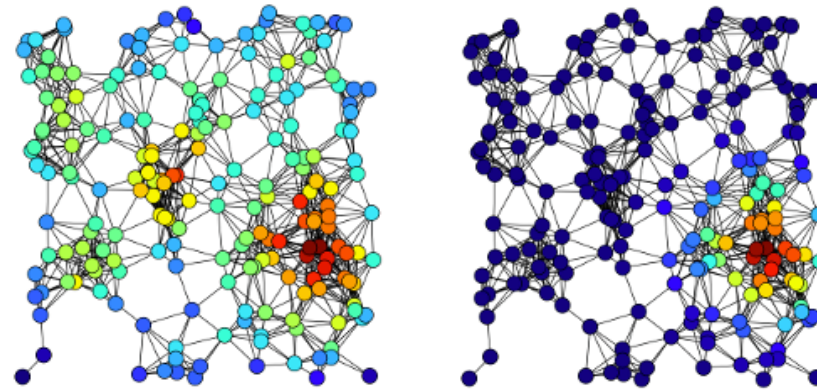


brain network

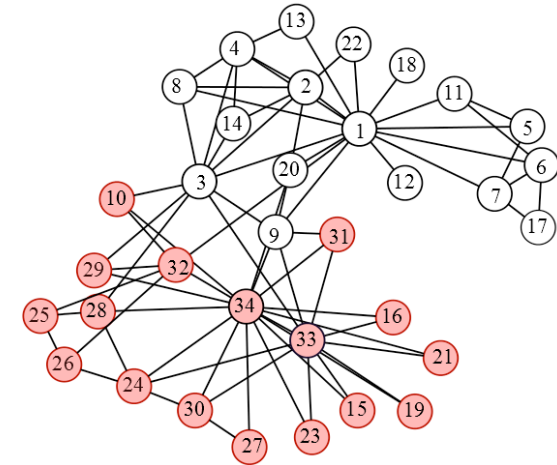
graphs provide mathematical representation of networks

The field of network science

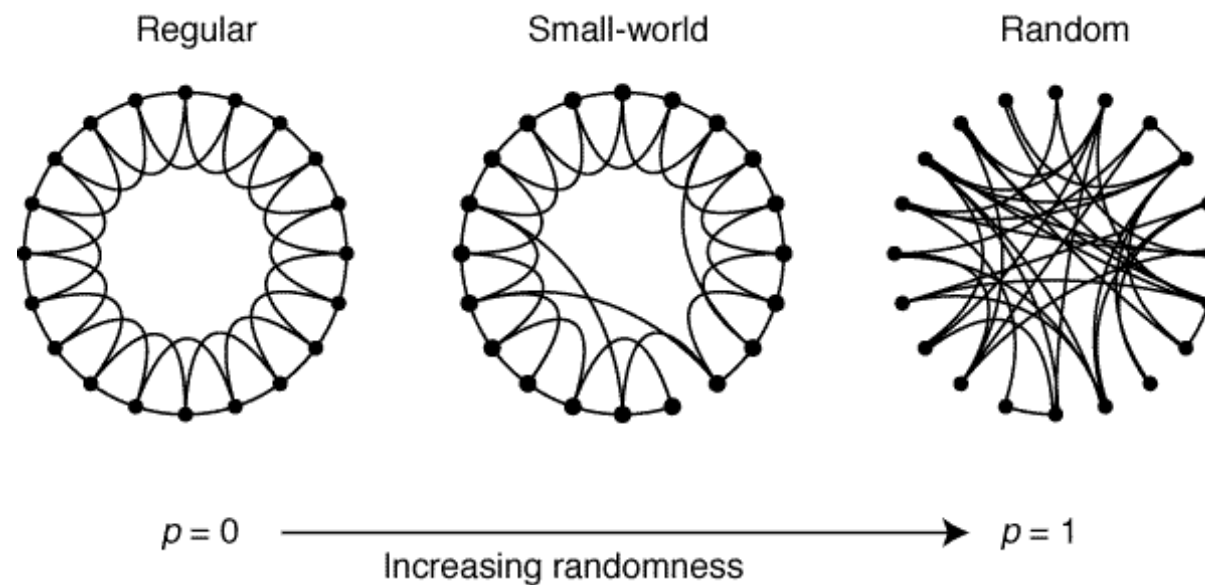
network
centrality



community
detection

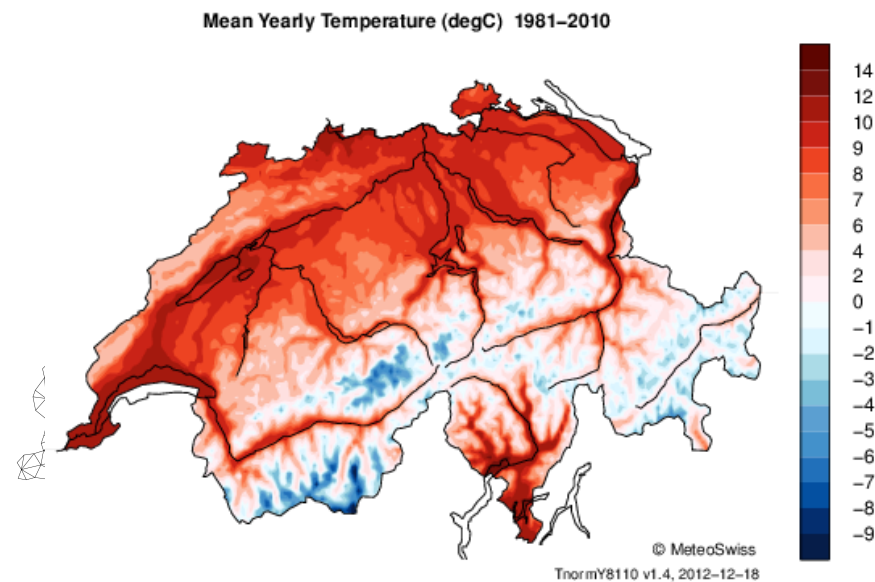


random graph
models



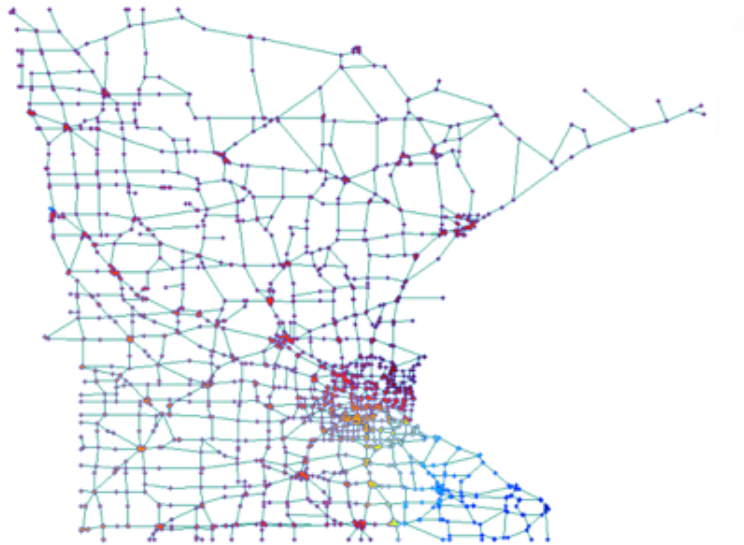
from **edge attributes** to **node attributes**
from **graphs** to **graph-structured data**

Graph-structured data are pervasive



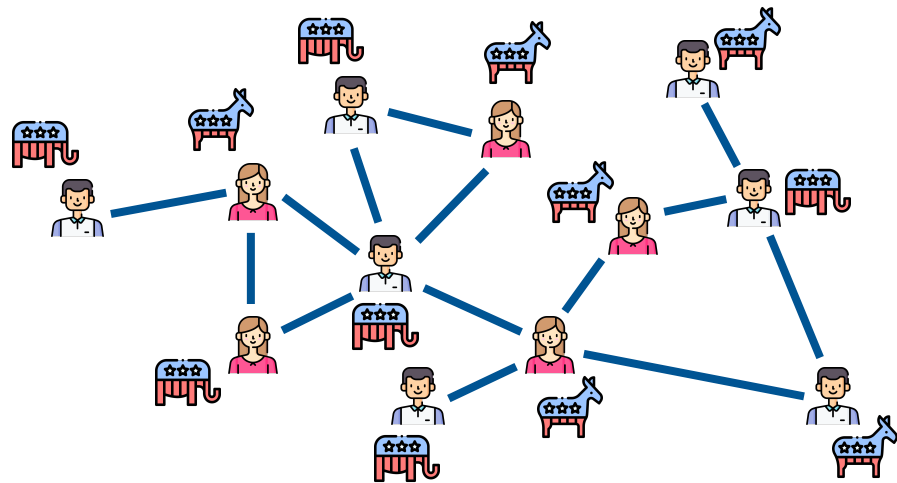
- nodes
 - geographical regions
- edges
 - geographical proximity between regions
- signal
 - temperature records in these regions

Graph-structured data are pervasive



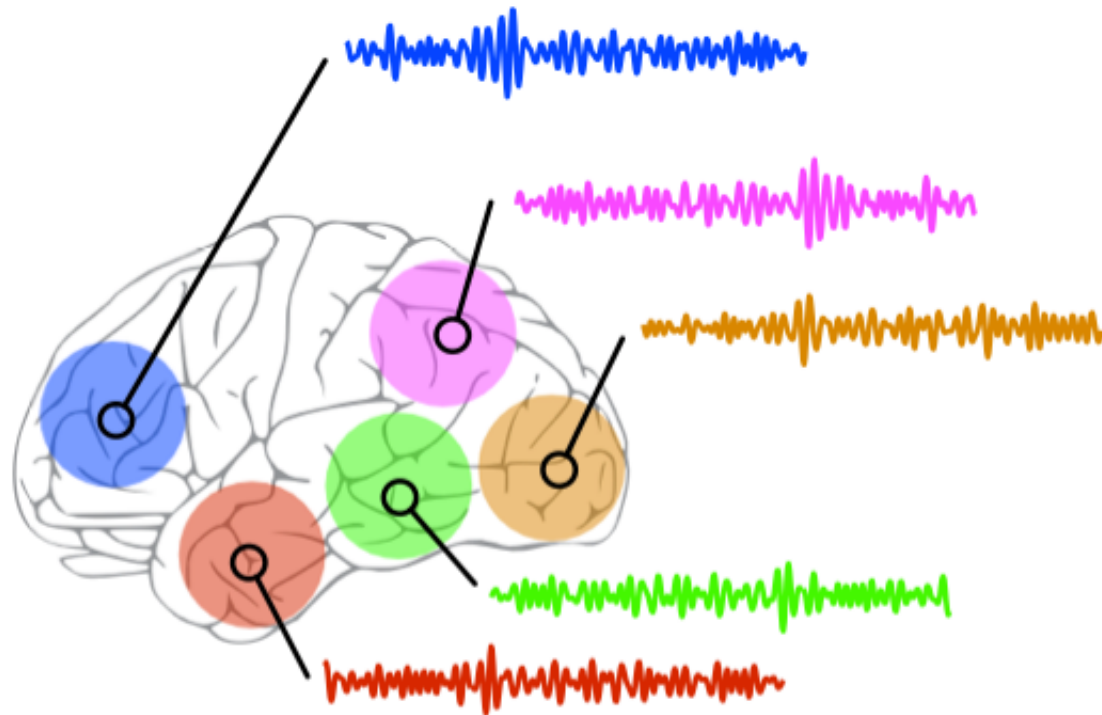
- nodes
 - road junctions
- edges
 - road connections
- signal
 - traffic congestion at junctions

Graph-structured data are pervasive



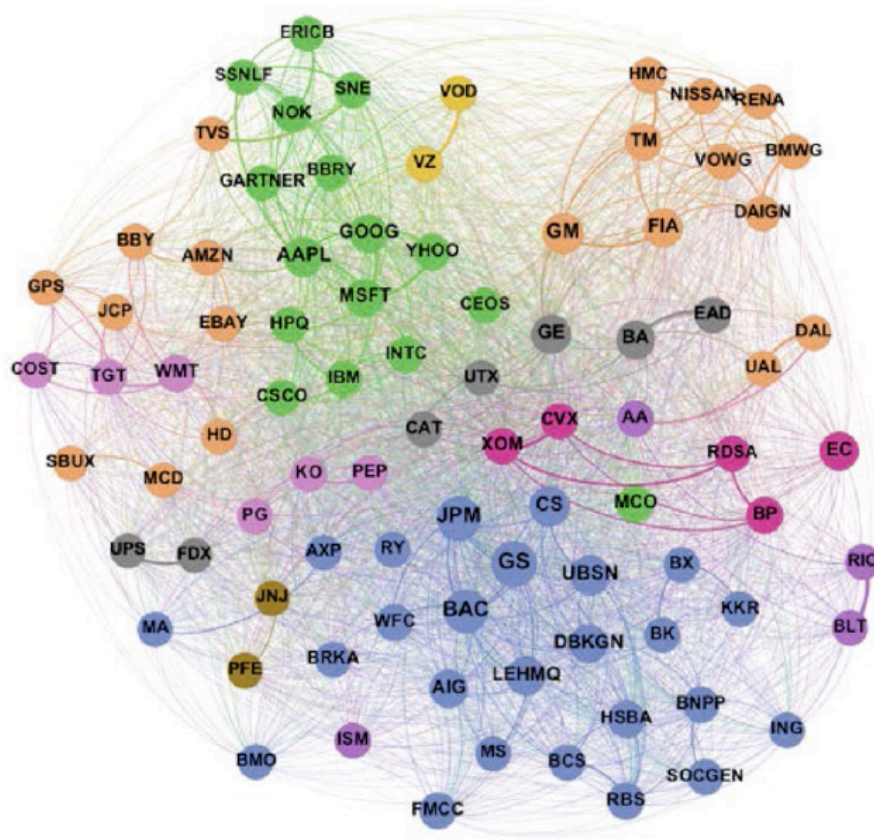
- nodes
 - individuals
- edges
 - friendship between individuals
- signal
 - political view

Graph-structured data are pervasive



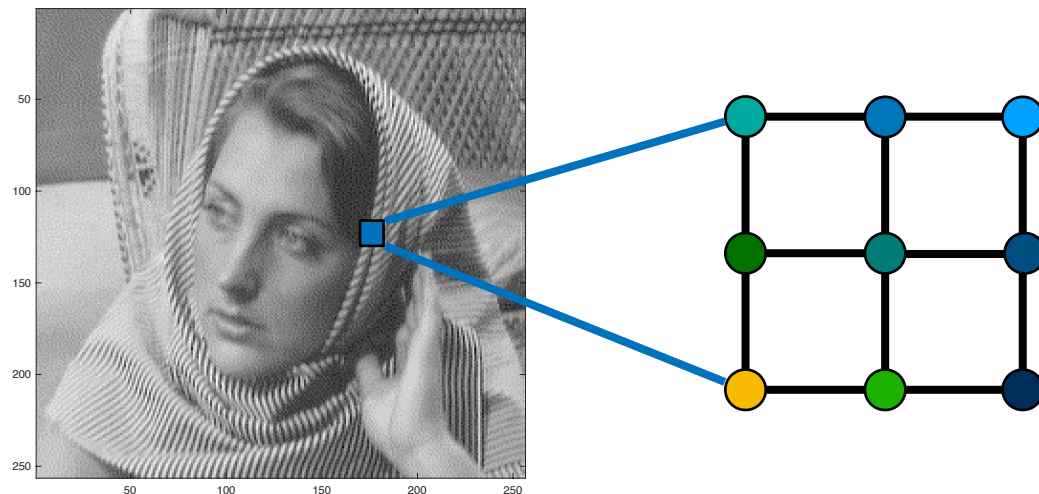
- nodes
 - brain regions
- edges
 - structural connectivity between brain regions
- signal
 - blood-oxygen-level-dependent (BOLD) time series

Graph-structured data are pervasive



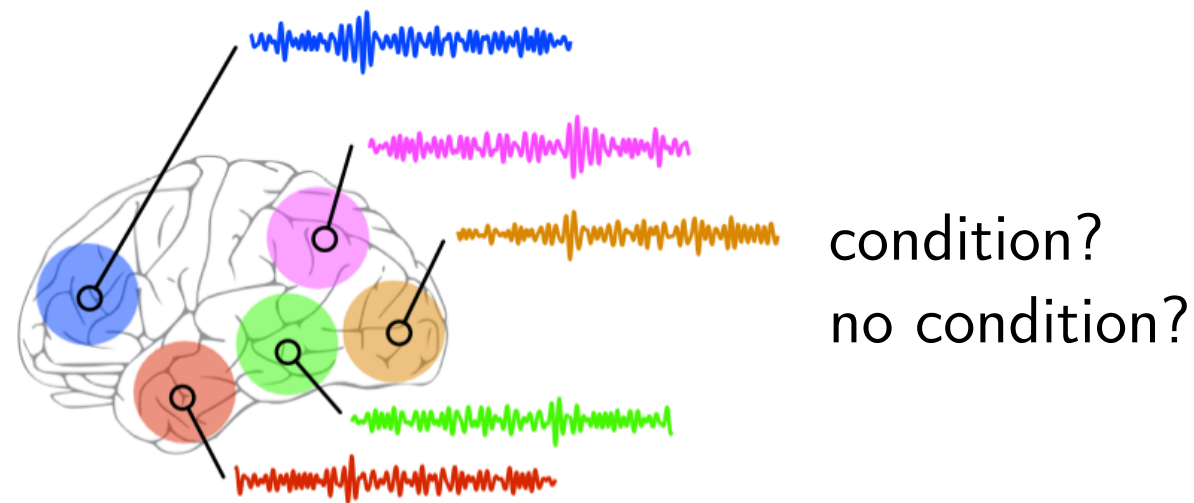
- nodes
 - companies
- edges
 - co-occurrence of companies in financial news
- signal
 - stock prices of these companies

Graph-structured data are pervasive



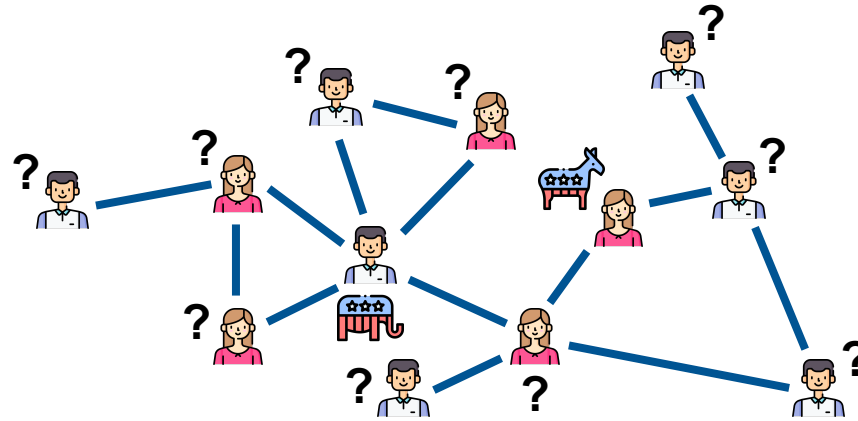
- nodes
 - pixels
- edges
 - spatial proximity between pixels
- signal
 - pixel values

Learning with graph-structured data



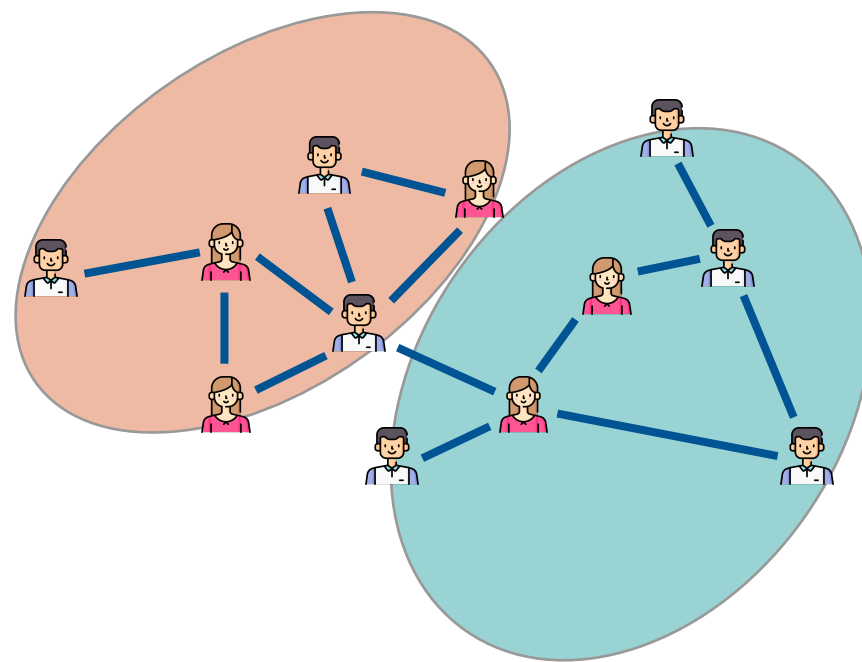
(supervised) graph-level classification

Learning with graph-structured data



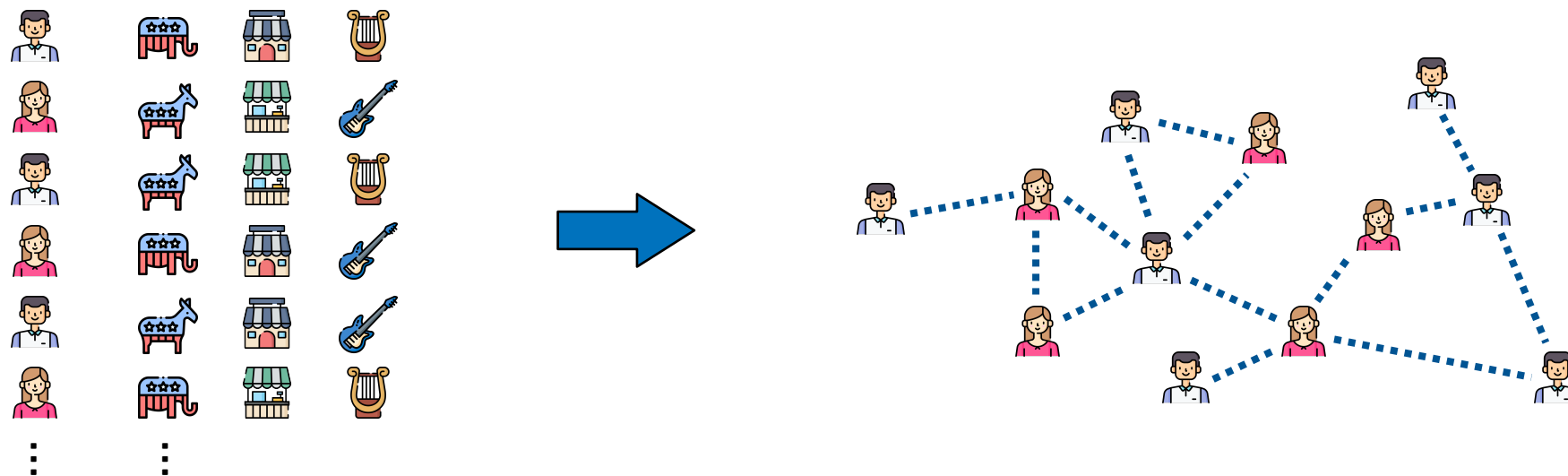
(semi-supervised) node-wise classification

Learning with graph-structured data



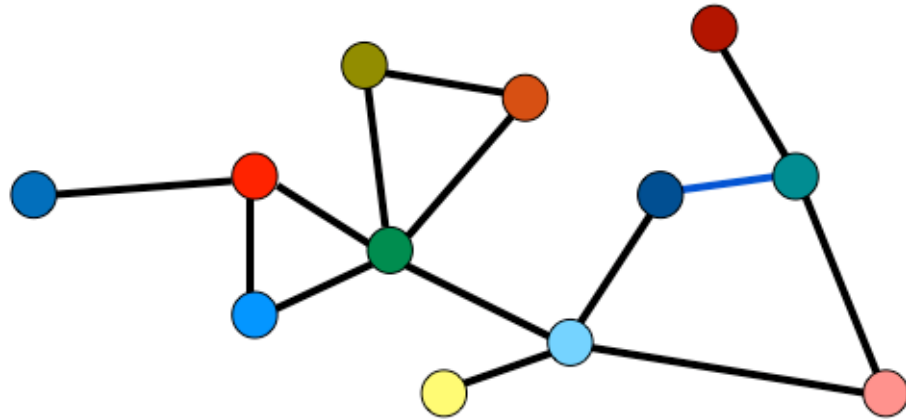
(unsupervised) clustering

Learning with graph-structured data



inferring graph topology from data

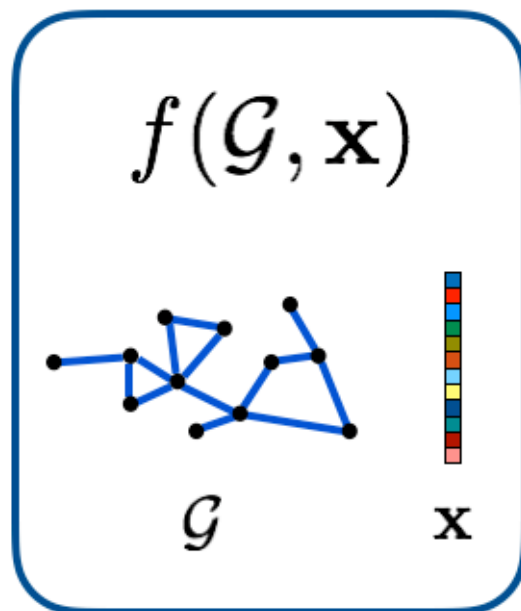
Graph-based machine learning



This tutorial:

- graph-structured data are **graph signals**
- how **graph signal processing** brings unique contribution to (graph-based) ML?

Graph-based ML



Tasks

Supervised learning
Unsupervised learning
Reinforcement learning

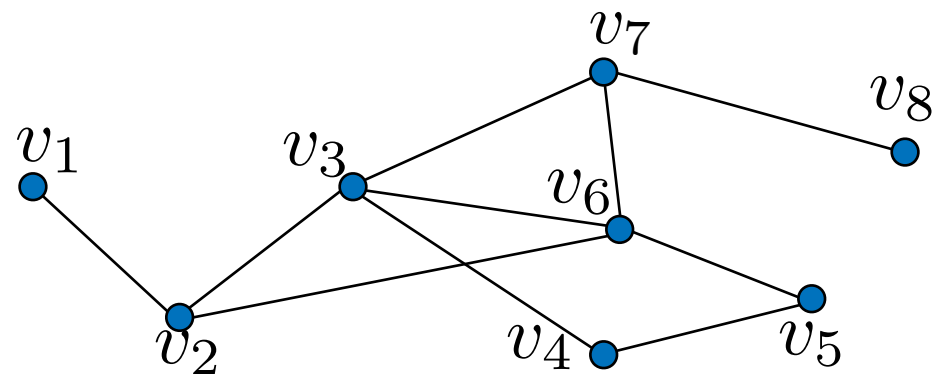
Challenges

Exploiting structure
Efficiency & Robustness
Model Interpretability

Outline

- Brief introduction to graph signal processing (GSP)
- Challenge I: GSP for exploiting data structure
- Challenge II: GSP for improving efficiency and robustness
- Challenge III: GSP for enhancing model interpretability
- Applications
- Summary, open challenges, and new perspectives

Graphs and graph Laplacian



weighted and undirected graph:

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

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

$$L = D - W \quad \text{equivalent to } \mathbf{G}!$$

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

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

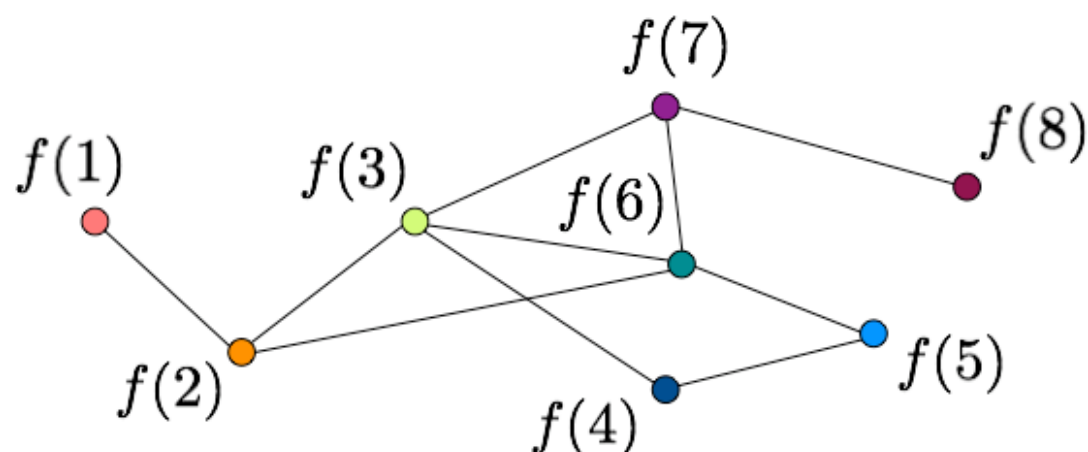
D

W

L

- symmetric
- off-diagonal entries non-positive
- rows sum up to zero

Graphs and graph Laplacian



graph signal $f : \mathcal{V} \rightarrow \mathbb{R}$

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

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

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

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

a measure of “smoothness”

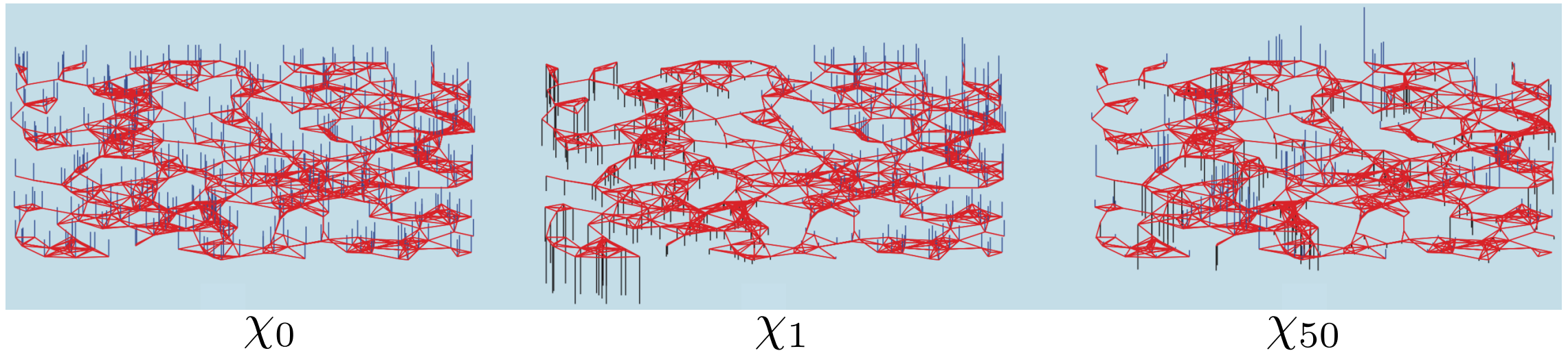
Graphs and graph Laplacian

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

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

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

Graph Fourier transform



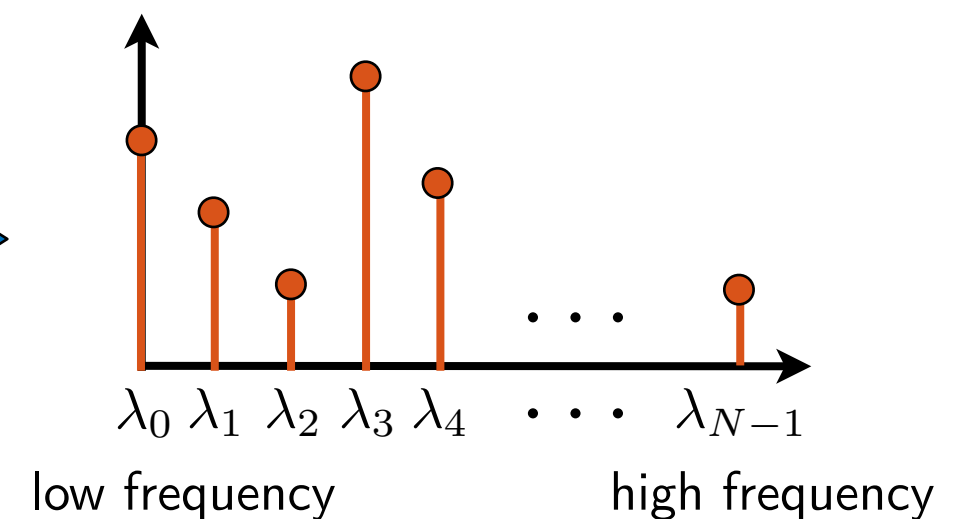
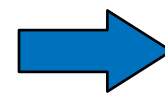
$$L = \chi \Lambda \chi^T$$

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

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

graph Fourier transform:

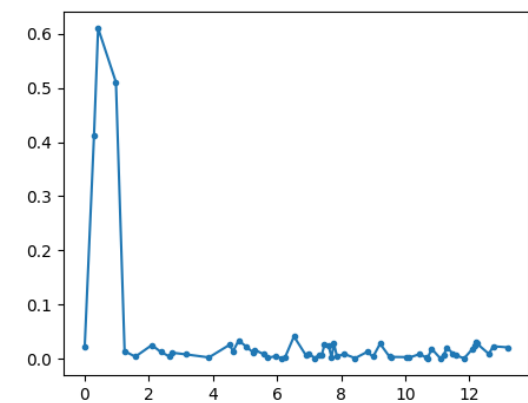
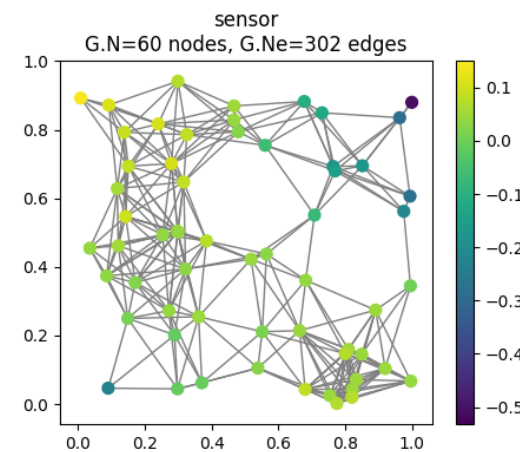
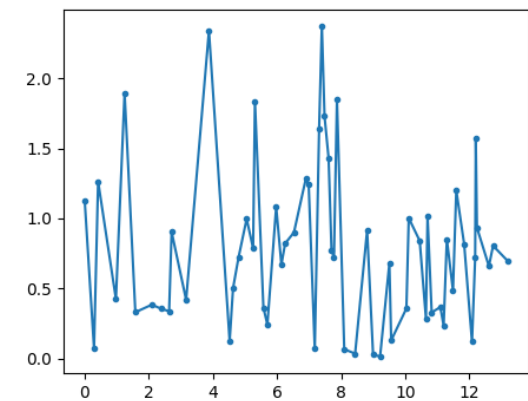
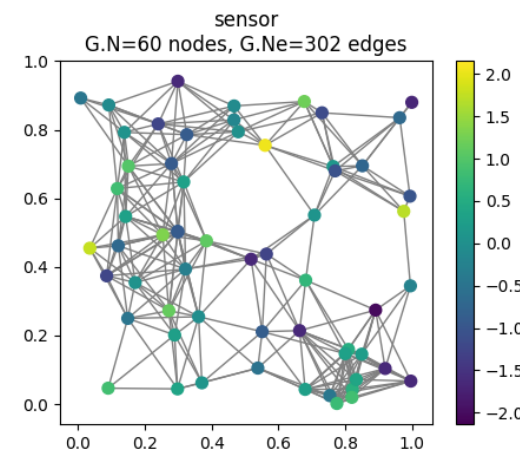
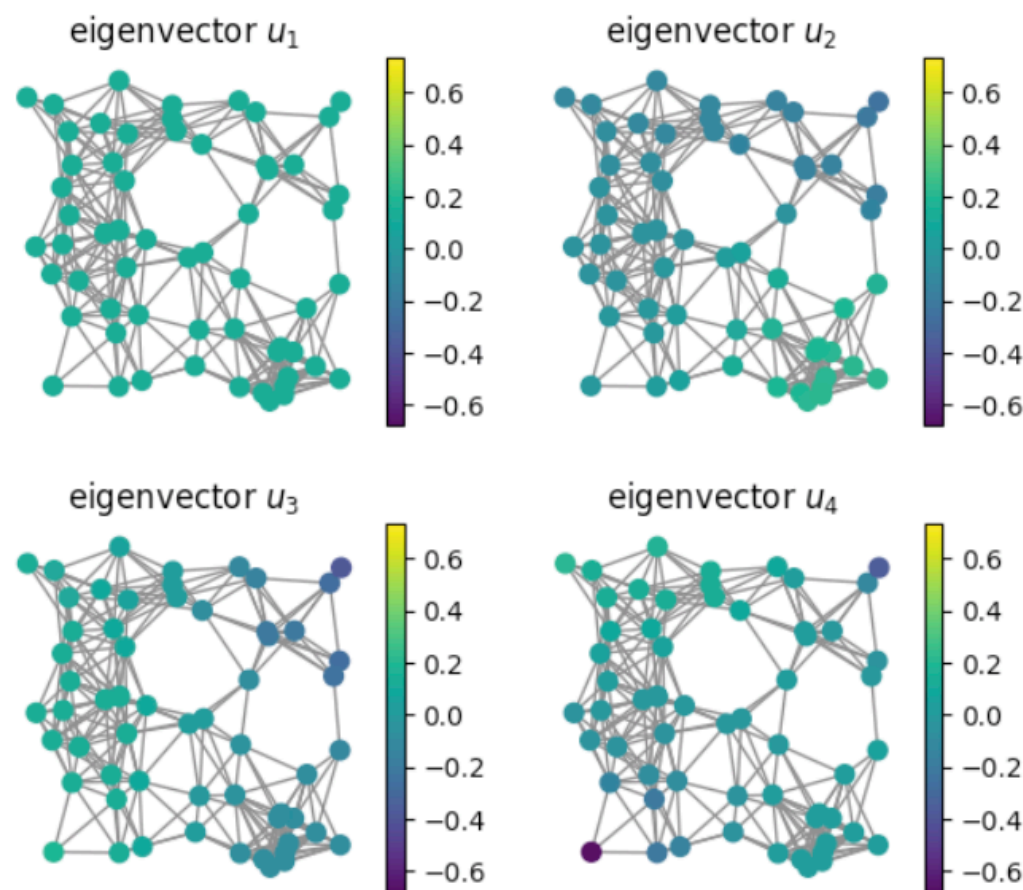
$$\hat{f}(\ell) = \langle \chi_\ell, f \rangle : \begin{bmatrix} | & & | \\ \chi_0 & \cdots & \chi_{N-1} \\ | & & | \end{bmatrix}^T \begin{bmatrix} | \\ f \\ | \end{bmatrix}$$



Graph Fourier transform

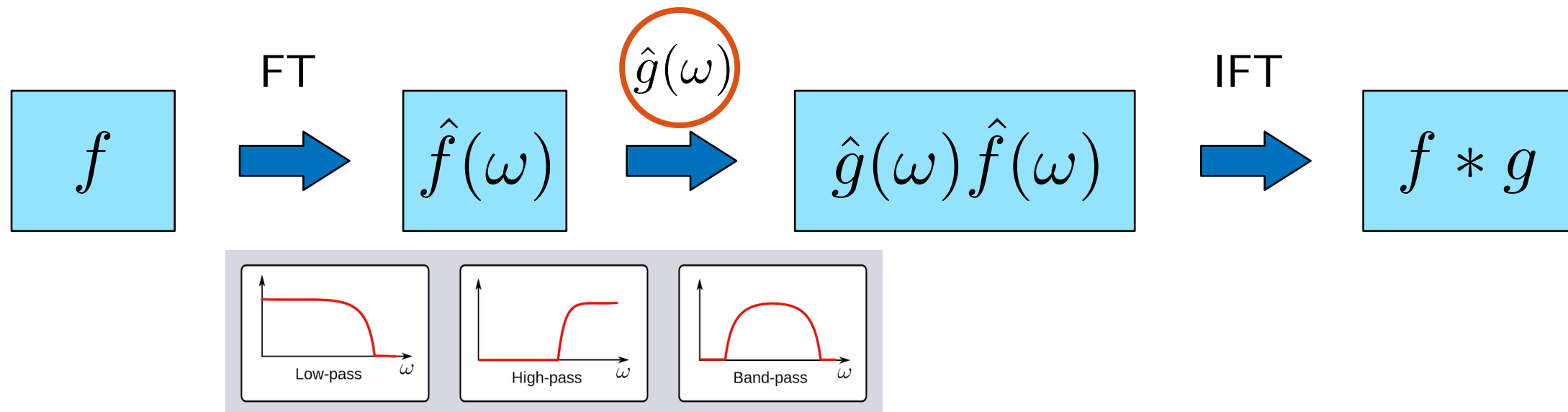
- Graph Fourier transform

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



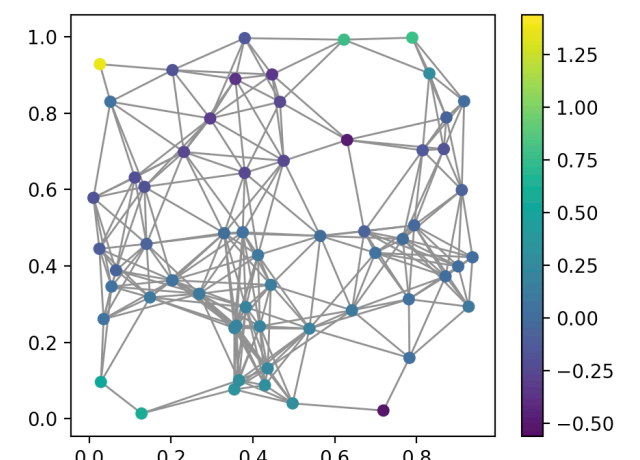
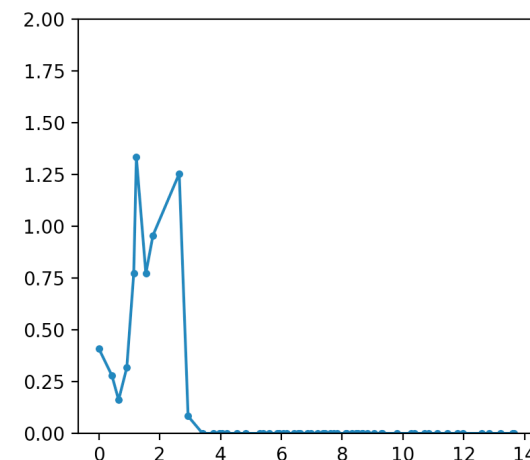
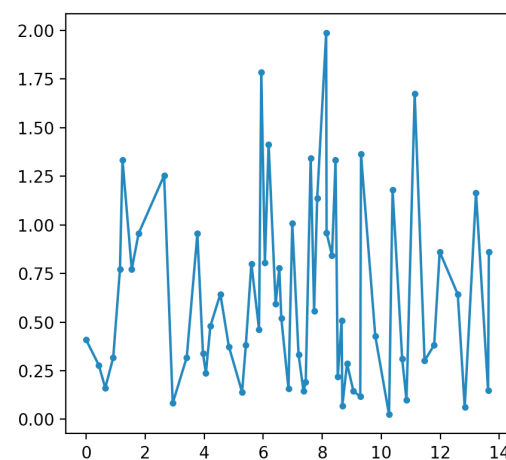
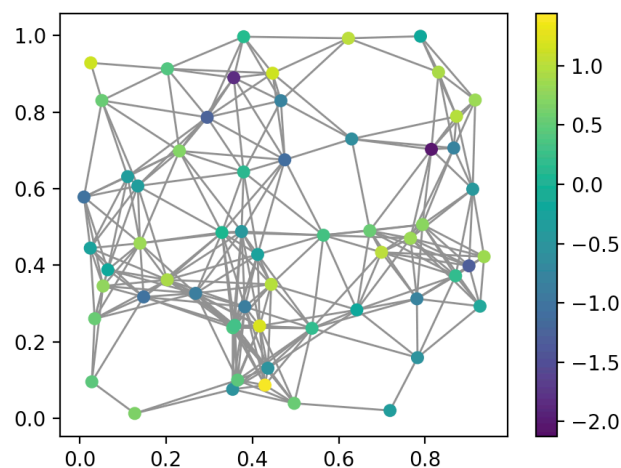
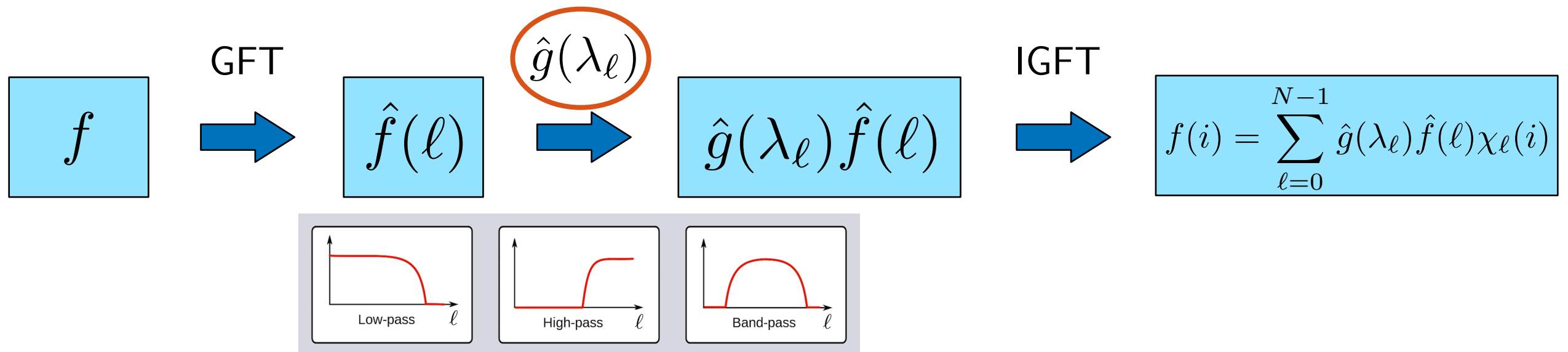
Classical frequency filtering

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



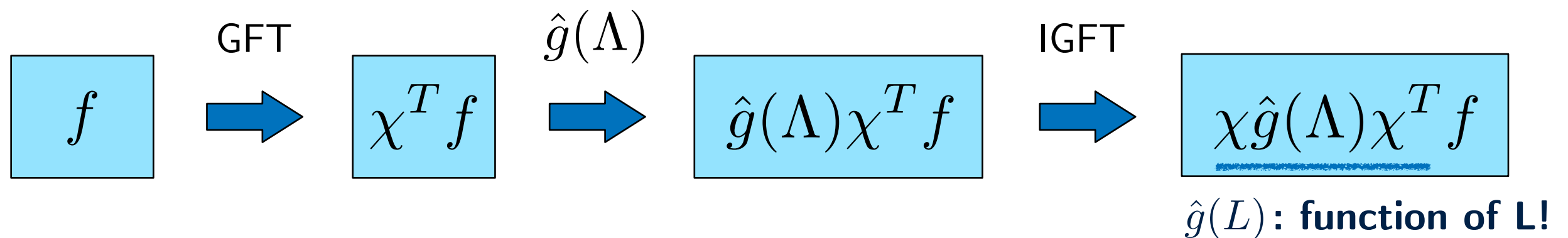
Graph spectral filtering

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



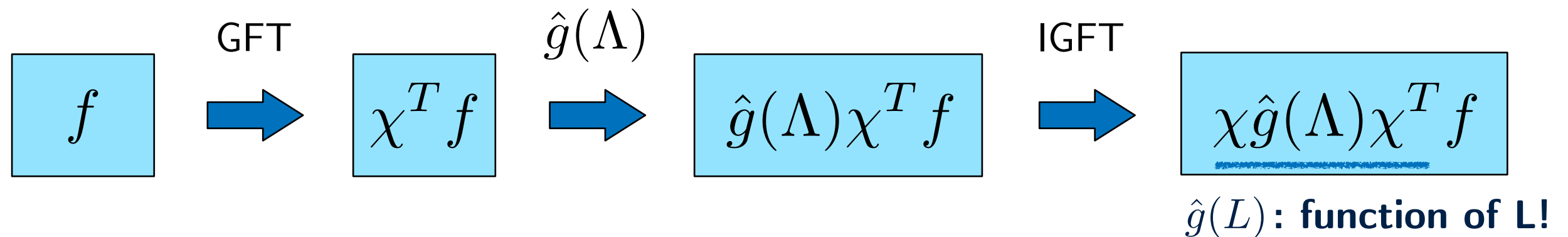
Graph transform/dictionary design

- 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 (more on this later)
- Closely related to kernels and regularisation on graphs

A practical example



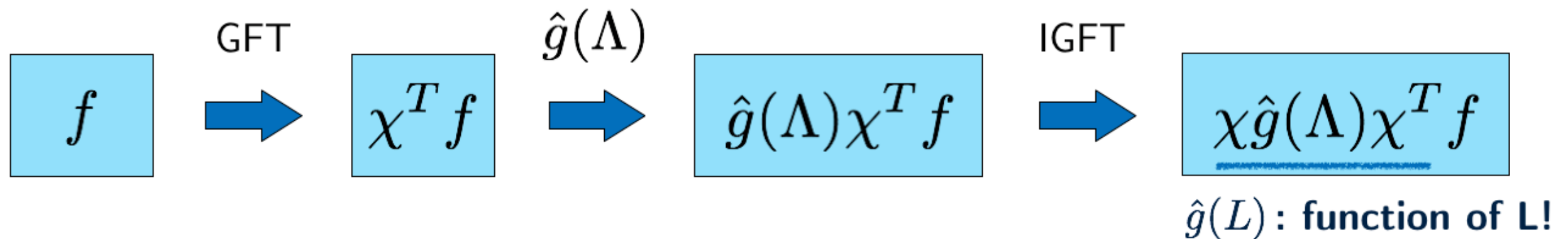
problem: we observe a noisy graph signal $f = y_0 + \eta$ and wish to recover y_0

$$y^* = \arg \min_y \{ \underbrace{\|y - f\|_2^2}_{\text{data fitting term}} + \underbrace{\gamma y^T L y}_{\text{"smoothness" assumption}} \}$$

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

**remove noise by low-pass filtering
in graph spectral domain!**

Graph transform/dictionary design



smoothing/low-pass filtering: $\hat{g}(L) = (I + \gamma L)^{-1} = \chi(I + \gamma \Lambda)^{-1} \chi^T$

**Graph-based
regularisation**

windowed kernel: windowed graph Fourier transform

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

**Graph filters
& transforms**

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

parametric kernel: $\hat{g}(L) = \sum_{k=0}^K \theta_j L^k = \chi \left(\sum_{k=0}^K \theta_j \Lambda^k \right) \chi^T$

**Learning models
on graphs**

GSP for machine learning

Graph-based regularisation

Graph filters & transforms

GSP-related learning models

Exploiting
structure

Efficiency &
Robustness

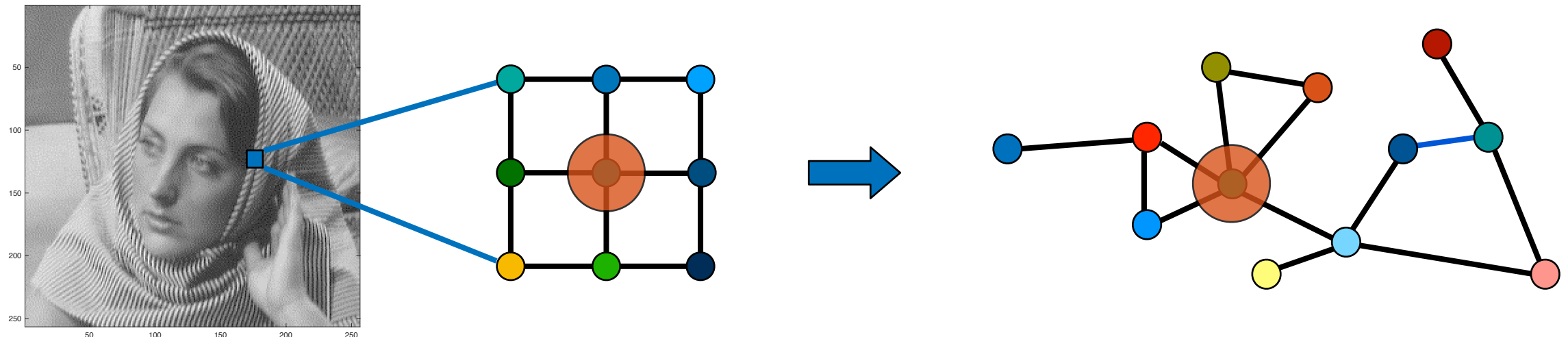
Model
Interpretability

- enable convolution & hierarchical modelling on graphs
- improve efficiency & robustness of (graph-based) ML models
- interpret data structure & learning models on graphs

Outline

- Brief introduction to graph signal processing (GSP)
- Challenge I: GSP for exploiting data structure
- Challenge II: GSP for improving efficiency and robustness
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- Applications
- Summary, open challenges, and new perspectives

GSP for exploiting data structure



- GSP enables definition of graph convolution
- GSP enriches design of graph convolutional models
- GSP facilitates hierarchical modelling on graphs

GSP for defining convolution on graphs

Convolution on graphs

classical convolution

time domain

$$(f * g)(t) = \int_{-\infty}^{\infty} f(t - \tau)g(\tau)d\tau$$

frequency domain

$$\widehat{(f * g)}(\omega) = \hat{f}(\omega) \cdot \hat{g}(\omega)$$

convolution on graphs

spatial (node) domain

$$f * g = \chi \hat{g}(\Lambda) \chi^T f = \hat{g}(L) f$$



graph spectral domain

$$\widehat{(f * g)}(\lambda) = ((\chi^T f) \circ \hat{g})(\lambda)$$



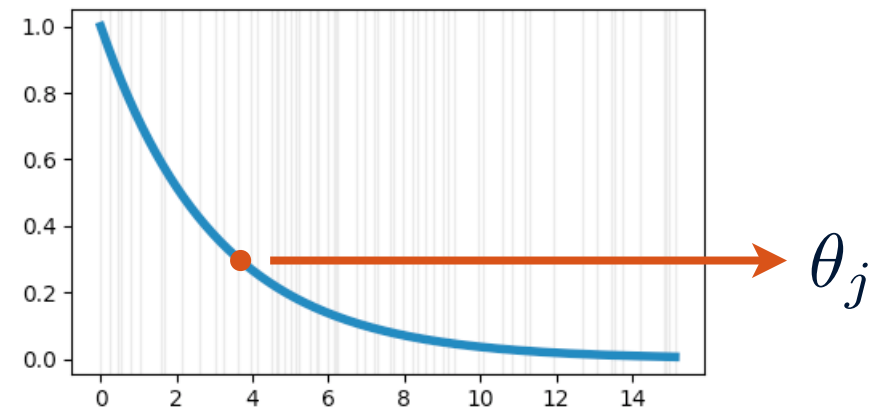
Convolution on graphs

$$f * g = \chi \hat{g}(\Lambda) \chi^T f = \hat{g}(L) f$$



learning a non-parametric filter:

$$\hat{g}_\theta(\Lambda) = \text{diag}(\theta), \quad \theta \in \mathbb{R}^N$$



- convolution expressed in the graph spectral domain
- no localisation in the spatial (node) domain

Convolution on graphs

$$f * g = \chi \hat{g}(\Lambda) \chi^T f = \hat{g}(L) f$$



parametric filter as polynomial of Laplacian

$$\hat{g}_\theta(\lambda) = \sum_{j=0}^K \theta_j \lambda^j, \quad \theta \in \mathbb{R}^{K+1}$$

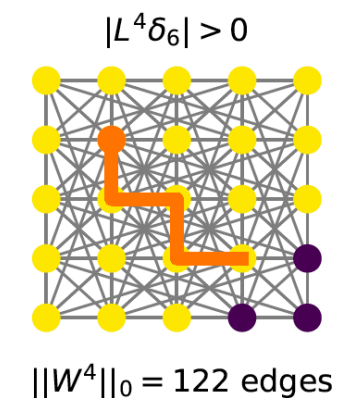
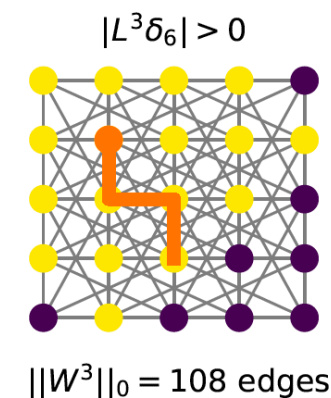
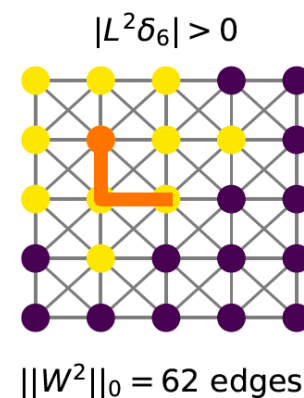
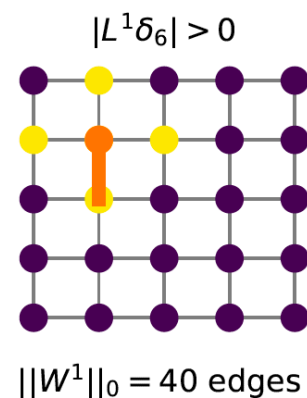
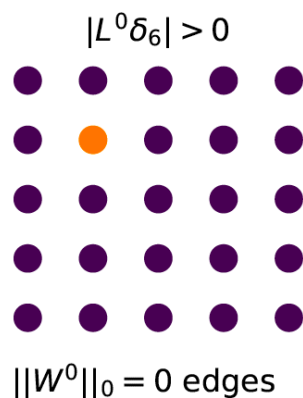
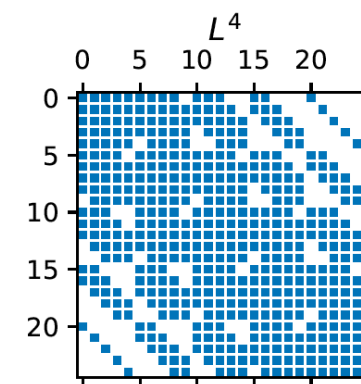
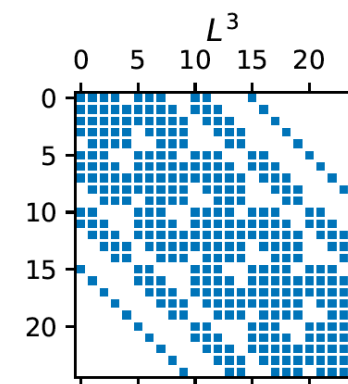
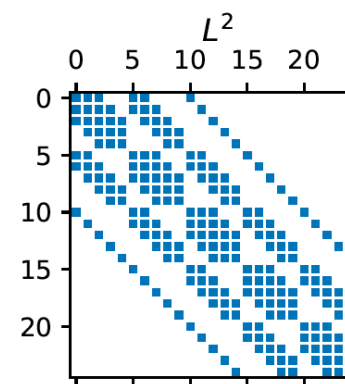
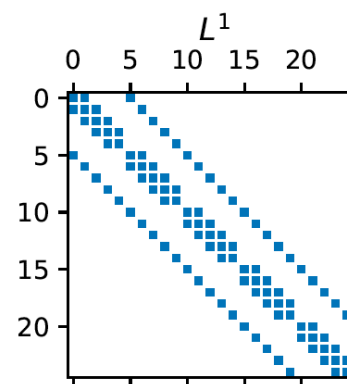
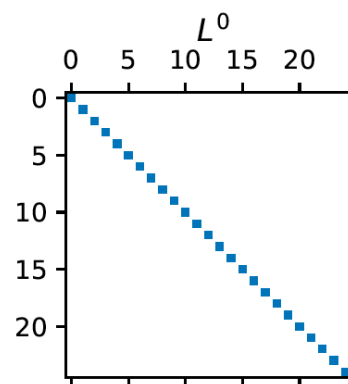


$$\hat{g}_\theta(L) = \sum_{j=0}^K \theta_j L^j$$

what do powers of graph Laplacian capture?

Powers of graph Laplacian

L^k defines the k -neighborhood



Localization: $d_G(v_i, v_j) > K$ implies $(L^K)_{ij} = 0$

(slide by Michaël Deferrard)

Convolution on graphs

$$f * g = \chi \hat{g}(\Lambda) \chi^T f = \hat{g}(L) f$$



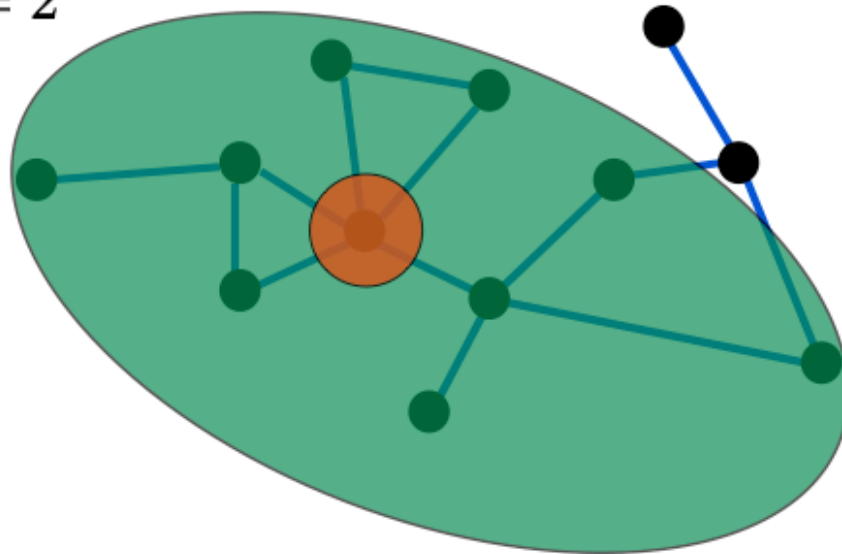
parametric filter as polynomial of Laplacian

$$\hat{g}_\theta(\lambda) = \sum_{j=0}^K \theta_j \lambda^j, \quad \theta \in \mathbb{R}^{K+1}$$



$$\hat{g}_\theta(L) = \sum_{j=0}^K \theta_j L^j \Rightarrow \sum_{j=0}^K \theta_j T_j(\tilde{L})$$

$K = 2$



- convolution is expressed in the graph spectral domain
- localisation within **K-hop** neighbourhood
- Chebyshev approximation using $\tilde{L} = 2L/\lambda_{N-1} - I$

Convolution on graphs

$$f * g = \chi \hat{g}(\Lambda) \chi^T f = \hat{g}(L) f$$



simplified polynomial

$$\hat{g}_\theta(L) = \sum_{j=0}^K \theta_j L^j \Rightarrow \sum_{j=0}^K \theta_j T_j(\tilde{L})$$

$$K = 1$$

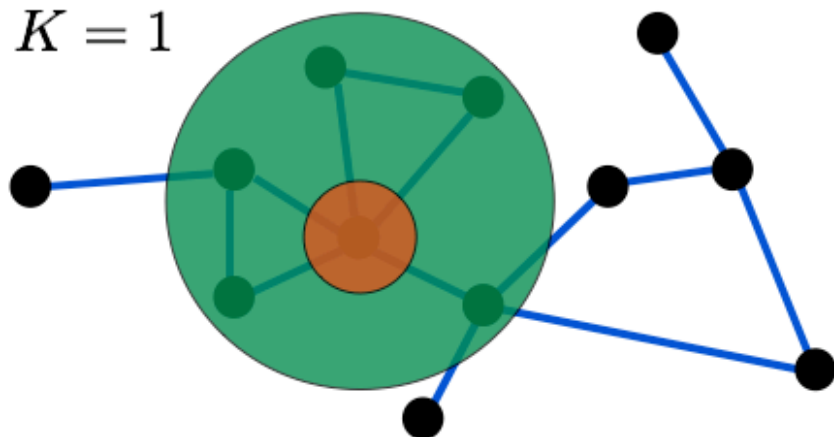
$$\lambda_{N-1} \approx 2$$



$$= \theta_0 I - \theta_1 (D^{-\frac{1}{2}} W D^{-\frac{1}{2}})$$

(localisation within **1-hop** neighbourhood)

$$K = 1$$



$$\alpha = \theta_0 = -\theta_1$$



$$= \alpha (I + D^{-\frac{1}{2}} W D^{-\frac{1}{2}})$$

renormalisation



$$\Rightarrow \alpha (\tilde{D}^{-\frac{1}{2}} \tilde{W} \tilde{D}^{-\frac{1}{2}})$$

Convolution on graphs - Remarks

- Convolution is defined via the **graph spectral** domain...

$$f * g = \chi \hat{g}(\Lambda) \chi^T f = \hat{g}(L) f$$

- ...but can be implemented in the **spatial (node)** domain

$$y = \hat{g}_\theta(L) f = \alpha(\tilde{D}^{-\frac{1}{2}} \tilde{W} \tilde{D}^{-\frac{1}{2}}) f \quad \rightarrow \quad \text{simple neighbourhood averaging in Kipf and Welling 2017}$$

Convolution on graphs - Remarks

- Convolution in classical signal processing relies on the shift operator

$$(f * g)(t) = \int_{-\infty}^{\infty} \boxed{f(t - \tau)} g(\tau) d\tau$$

- Notion of shift by a graph shift operator (e.g., adjacency/Laplacian matrix)

$$\boxed{Sf} \quad \rightarrow \quad g(S)f = \sum_{k=0}^K \theta_k \boxed{S^k f}$$

- spatial definition of convolution that resembles an FIR filter (on graphs)
- motivated from a **spatial** perspective, but has a **spectral** interpretation via eigendecomposition of S

Convolution on graphs - Remarks

- Convolution can also be interpreted as a weighted summation

$$(f * g)(t) = \int_{-\infty}^{\infty} f(\tau) g(t - \tau) d\tau$$

- Spatial generalisation of convolution in non-Euclidean domain

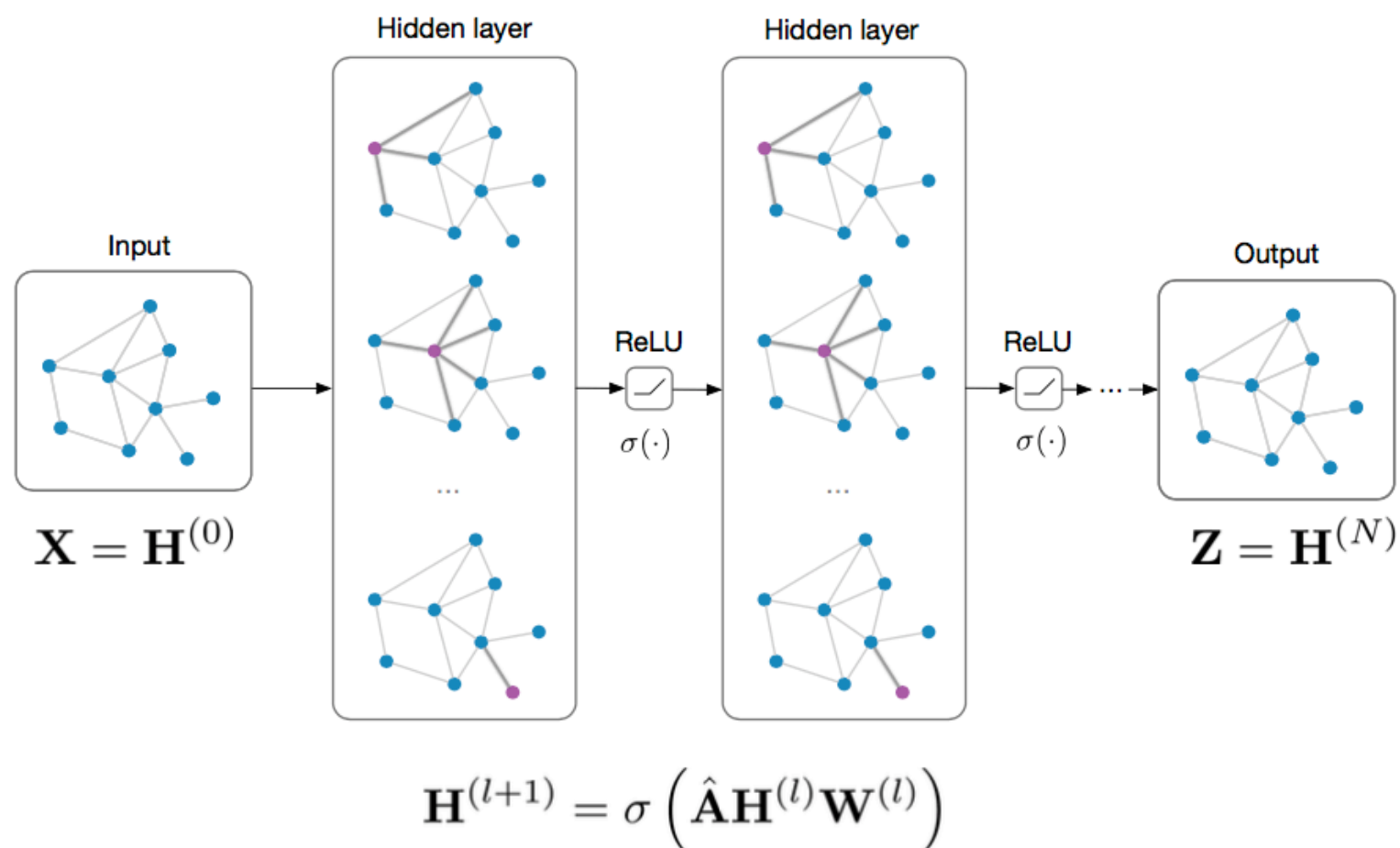
$$D(x)f = \int_{\mathcal{X}} f(x') u(x, x') dx' \quad \rightarrow \quad D(v)f = \sum_v f(v') u(v, v')$$

- weighting function $u(v, v')$ determines relative importance of neighbours

Graph convolutional networks

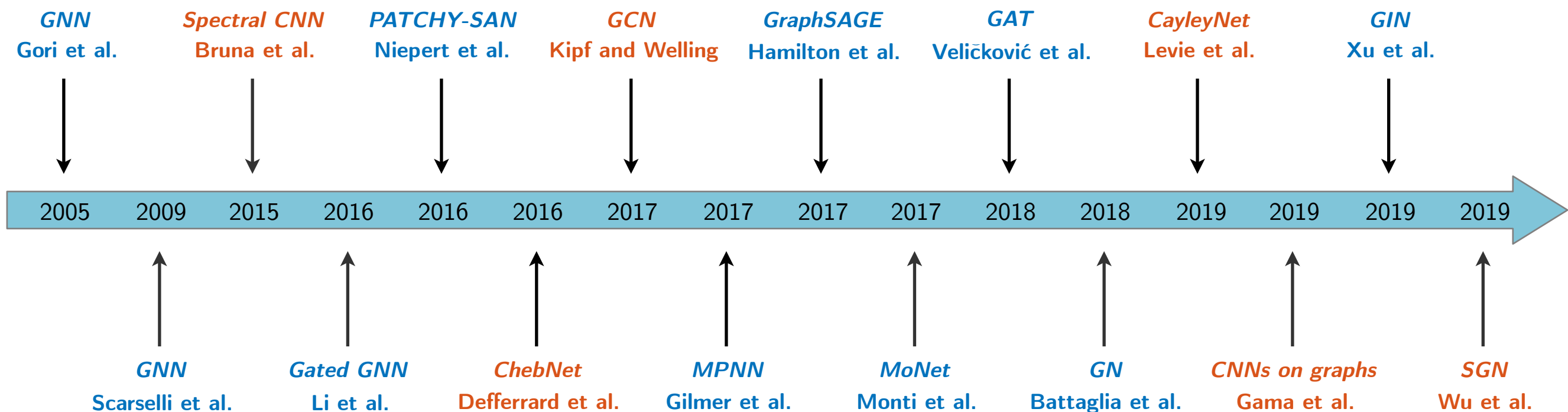
- Convolution on graphs leads to graph convolutional networks (GCNs)...

$$\hat{g}_{\theta^{(k+1)}}(L) \left(\text{ReLU}(\hat{g}_{\theta^{(k)}}(L)f) \right)$$



Graph neural networks

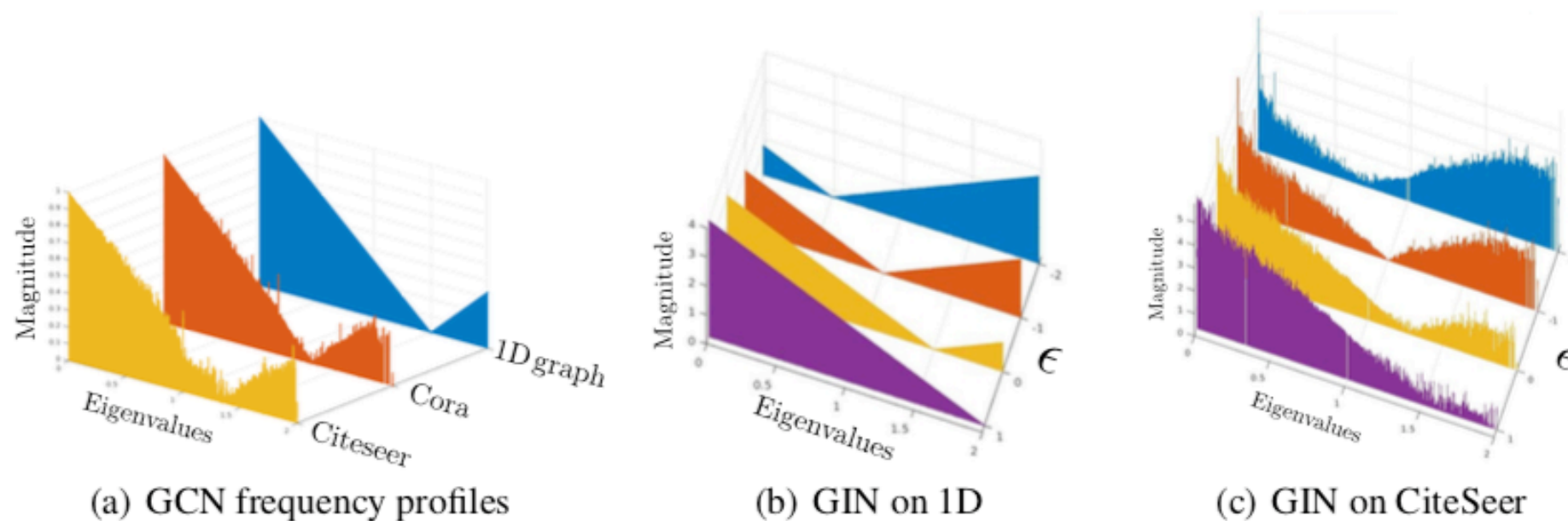
- ...and more generally graph neural networks (GNNs)



- **spatial** vs **spectral** designs

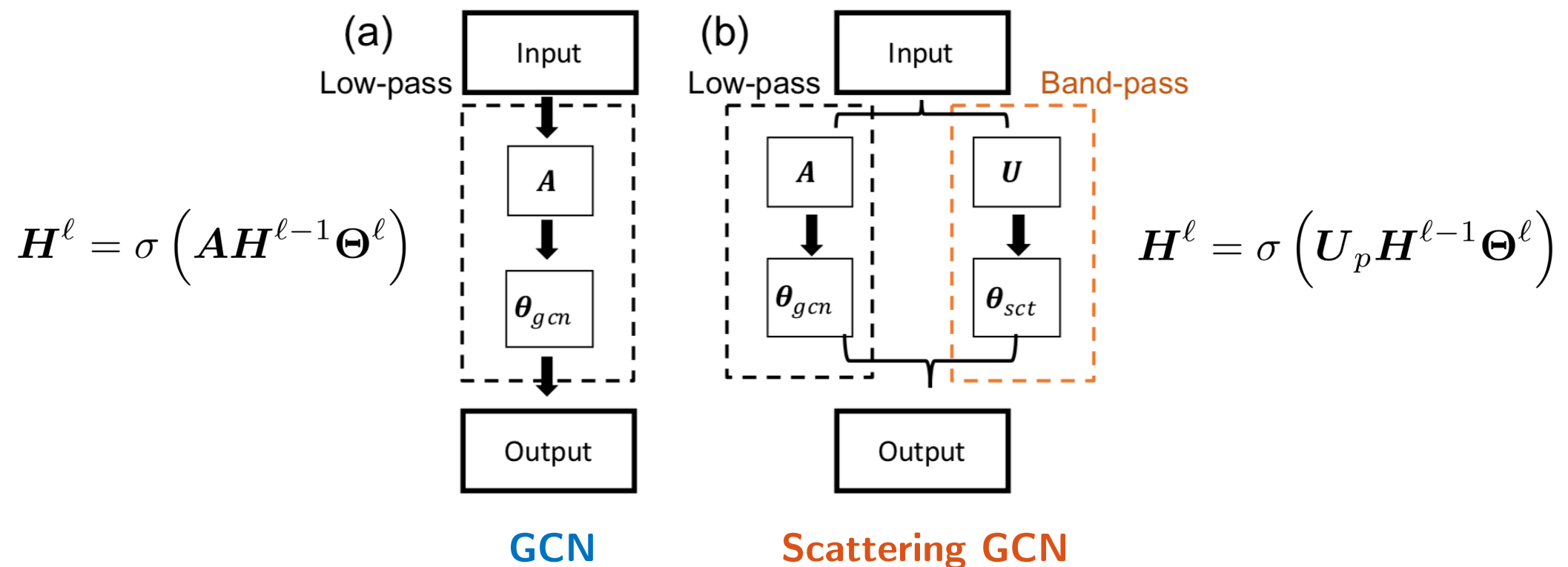
GSP for enriching graph convolutional models

Expressive power of GNNs



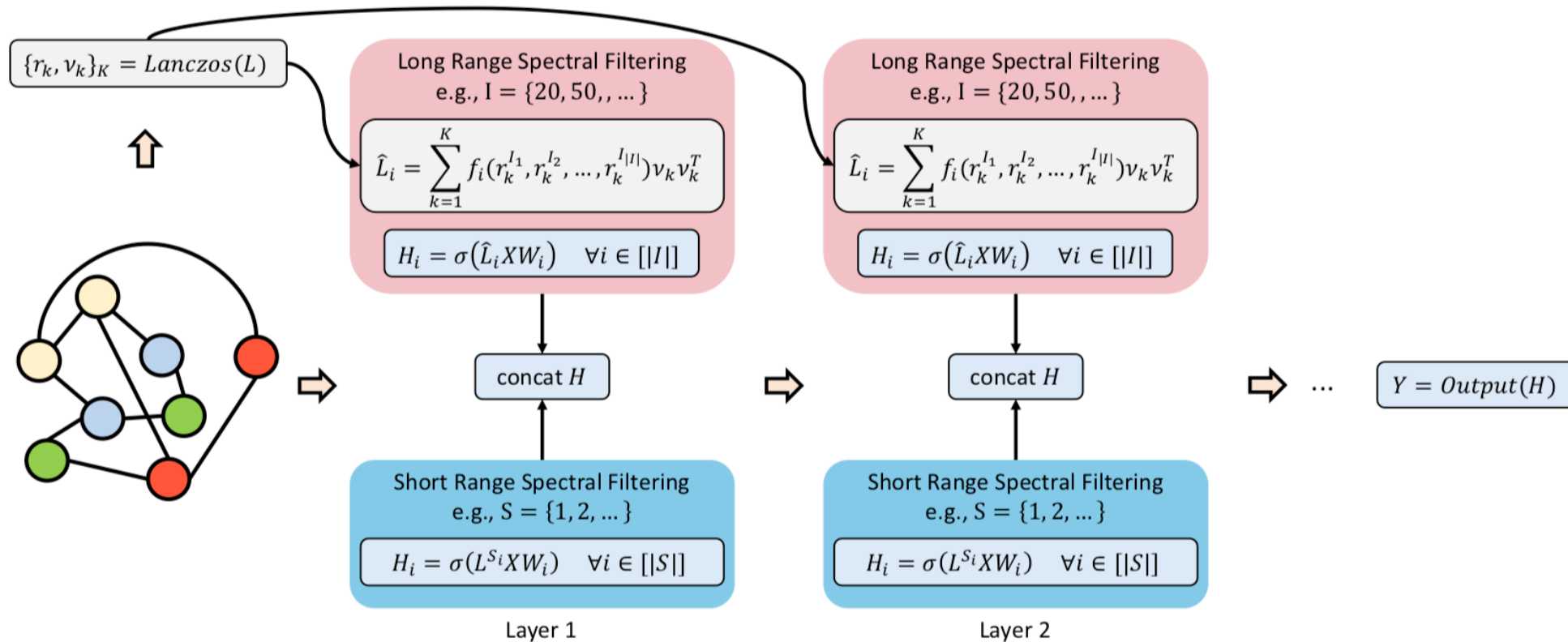
- convolutional layers in various GNN models can be understood as graph filters of different spectral profiles
- focusing on low-frequency information may lead to over-smoothing

Beyond low-frequency information



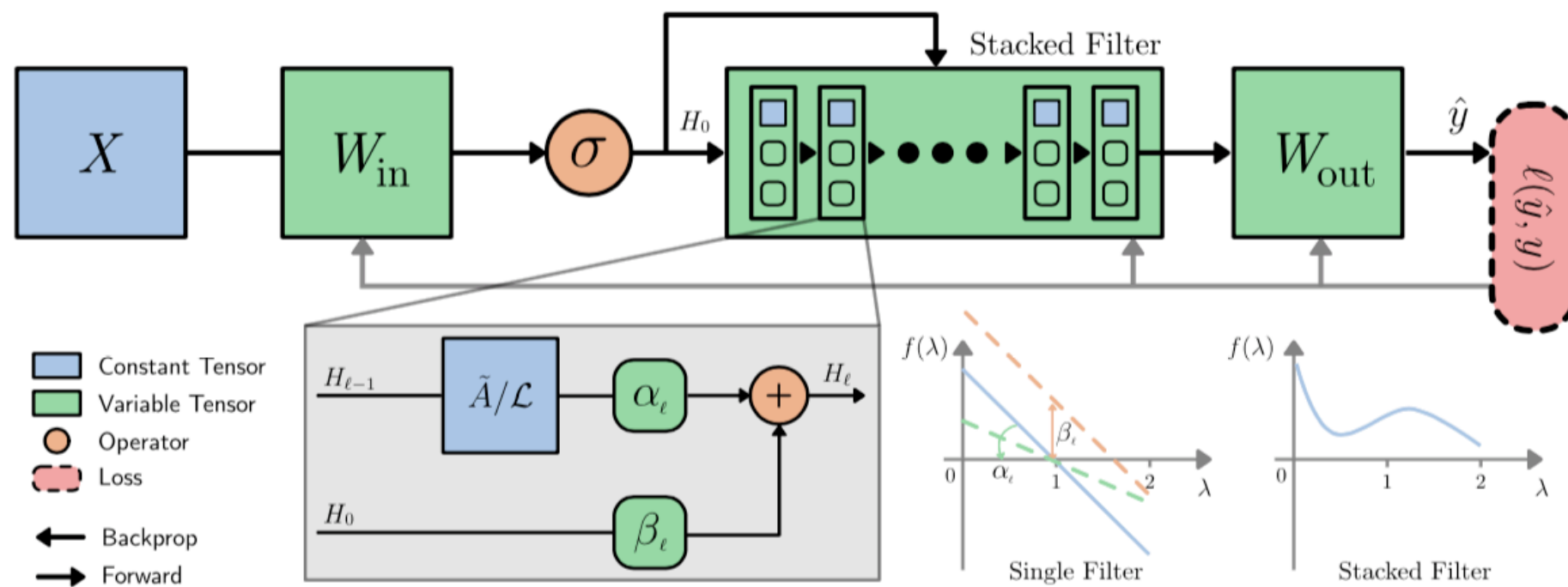
- combine low-pass operations based on GCN with band-pass operations based on geometric scattering (Min et al. 2020)
- combine low-pass and high-pass filtering (Bo et al. 2021)

Beyond low-frequency information



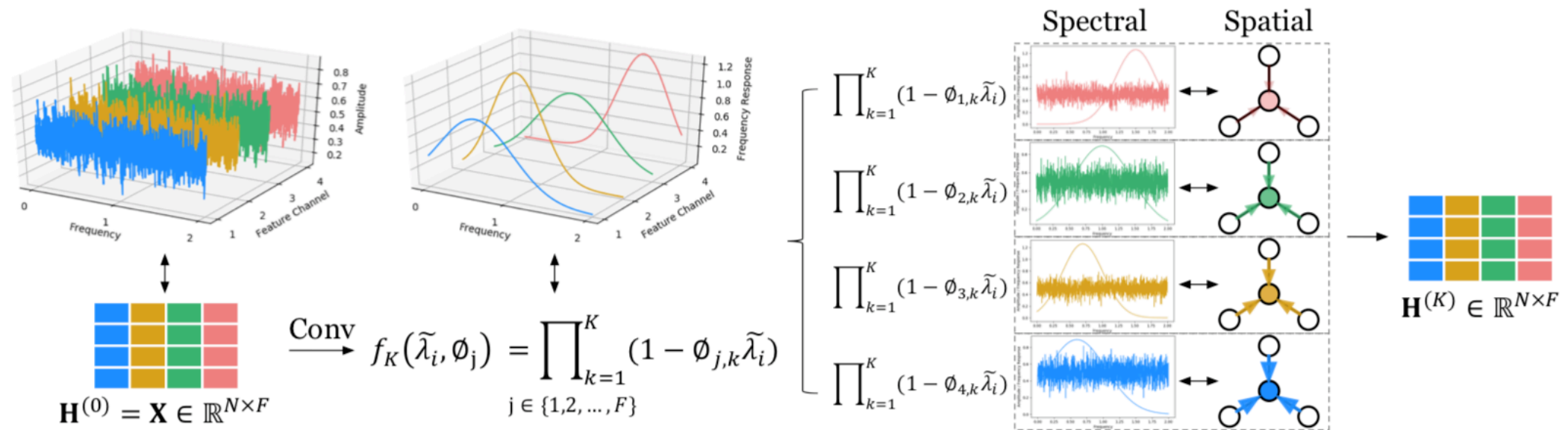
- combine short-range and long-range filtering
- long-range filtering facilitated by low-rank approximation to affinity matrix based on Lanczos algorithm
- learnable spectral filters based on the approximation

Adaptive filters



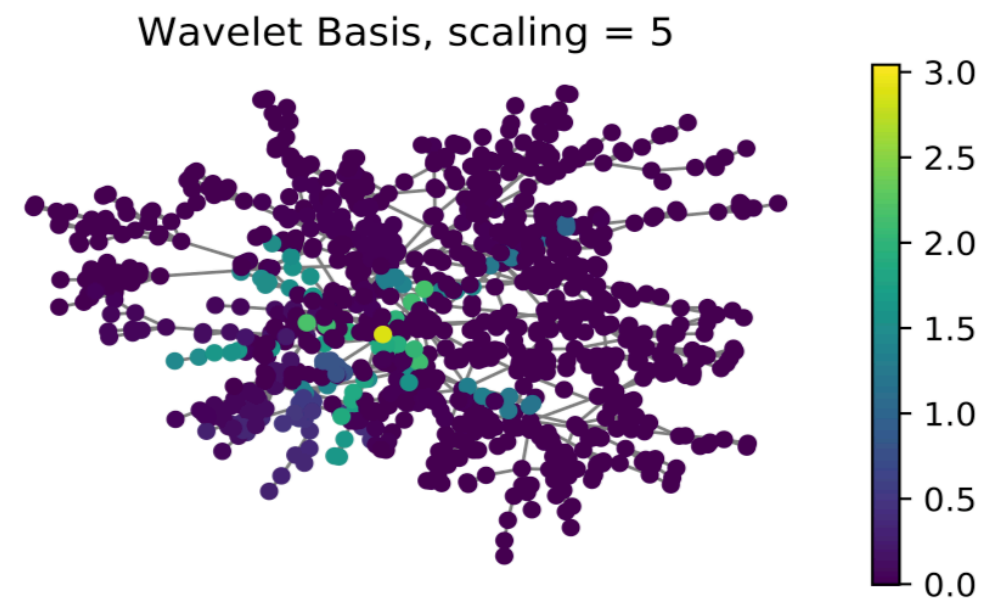
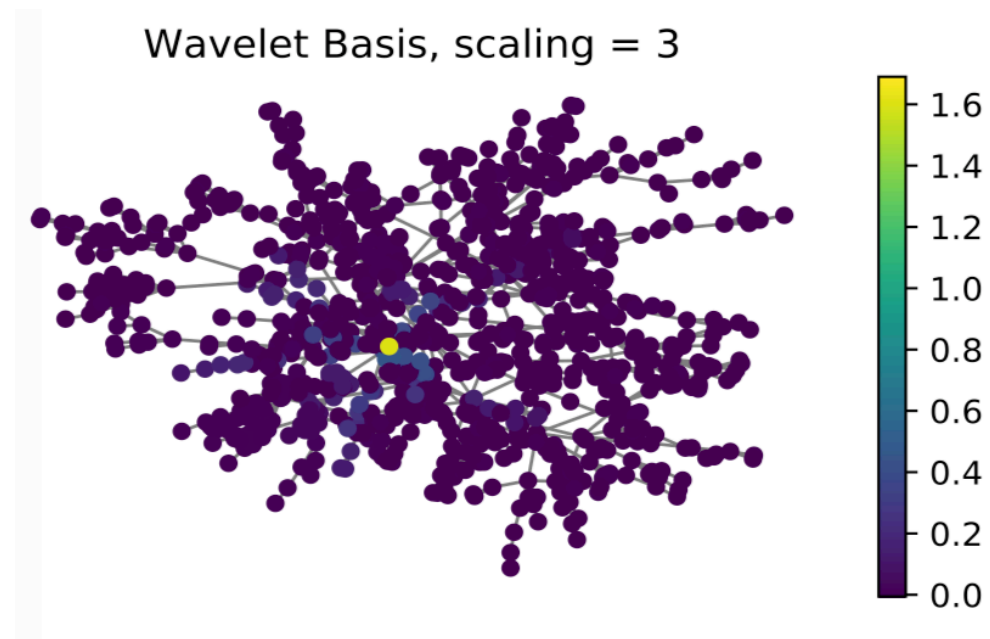
- stack graph filters with learnable filter parameters to build highly adaptive model

Adaptive filters



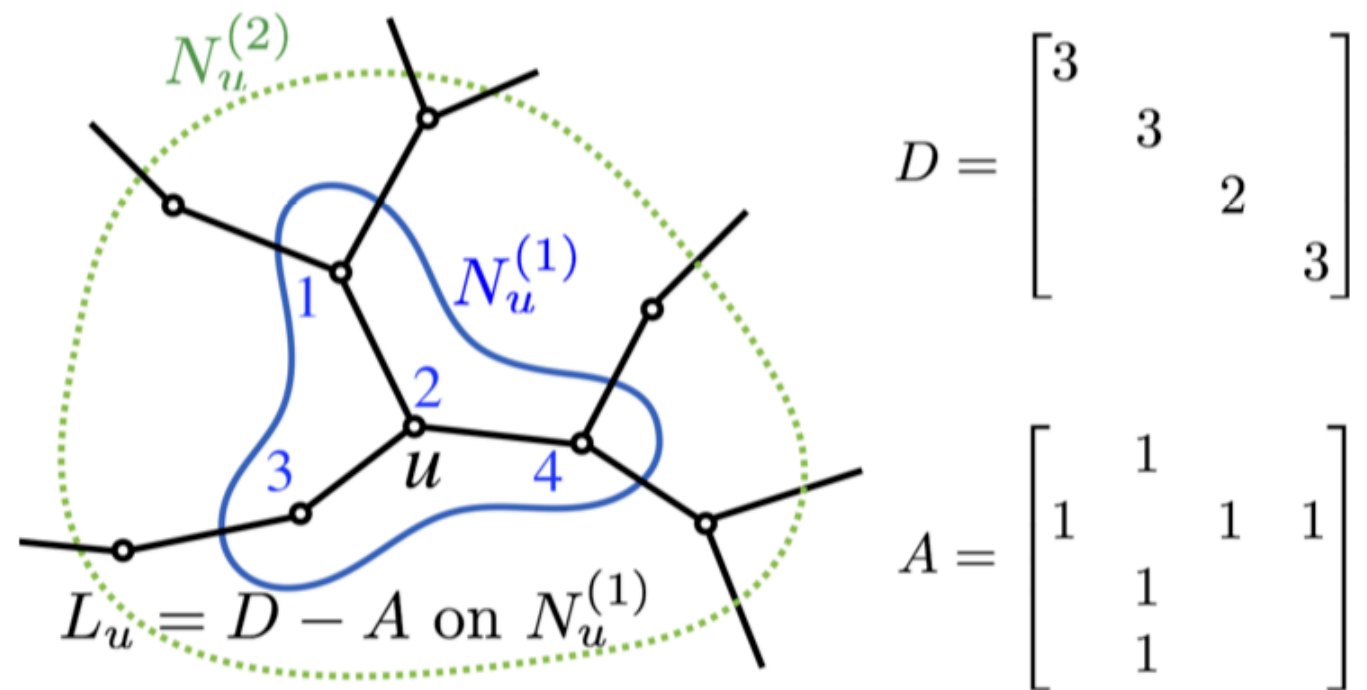
- stack learnable filters across network layers (removing nonlinearities at second and subsequence layers)
- learn separate adaptive filter for each feature channel

local basis filters



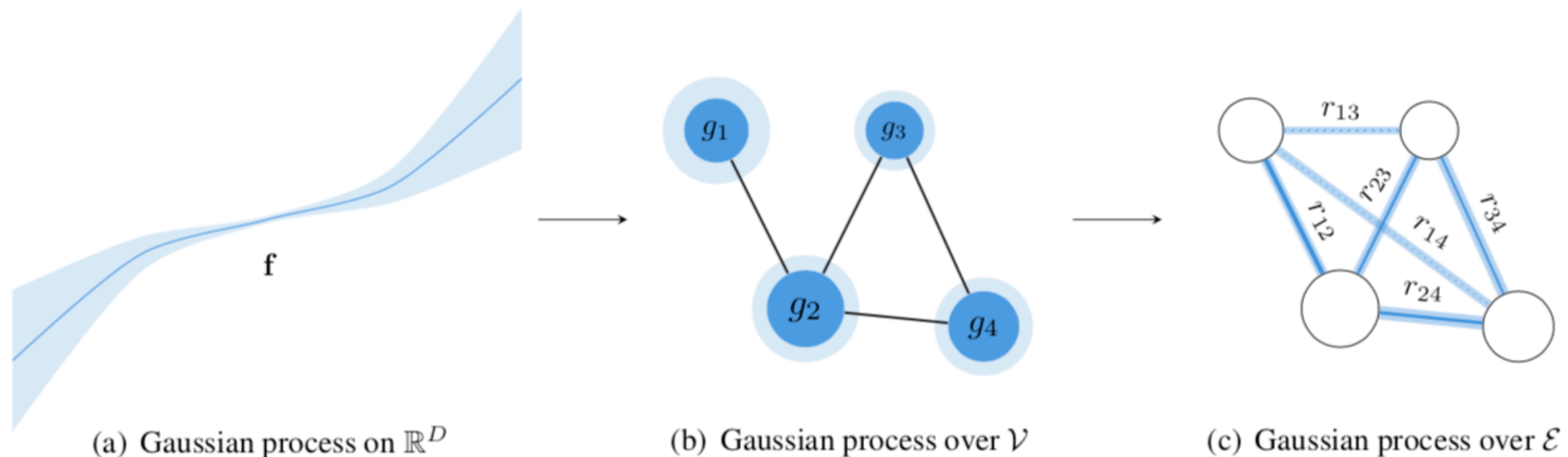
- replace Fourier basis with spectral graph wavelet basis to achieve localised convolution

local basis filters



- learnable local filters where localisation is imposed in spatial domain
- regularisation by local graph Laplacian to improve robustness

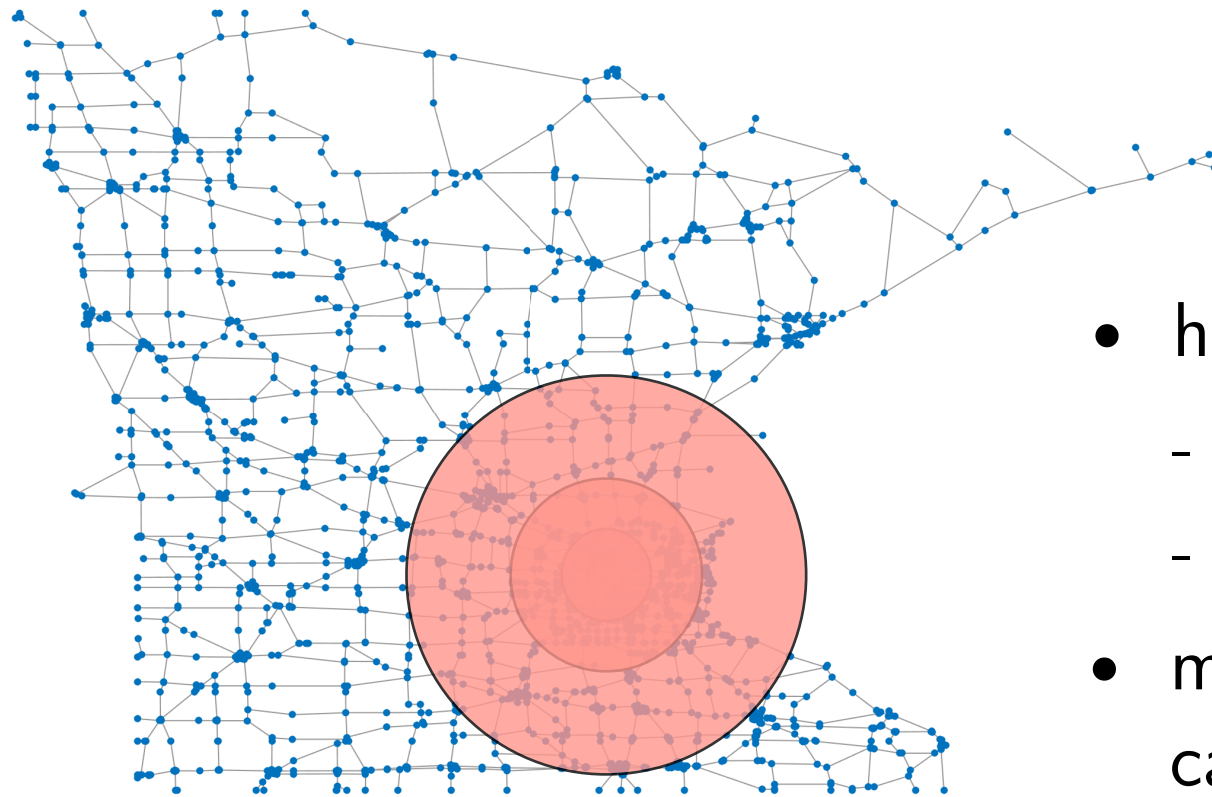
Graph convolutional Gaussian processes



- graph convolution enriches design of kernels associated with Gaussian processes (GPs)
- different formulations of convolution lead to different GP designs

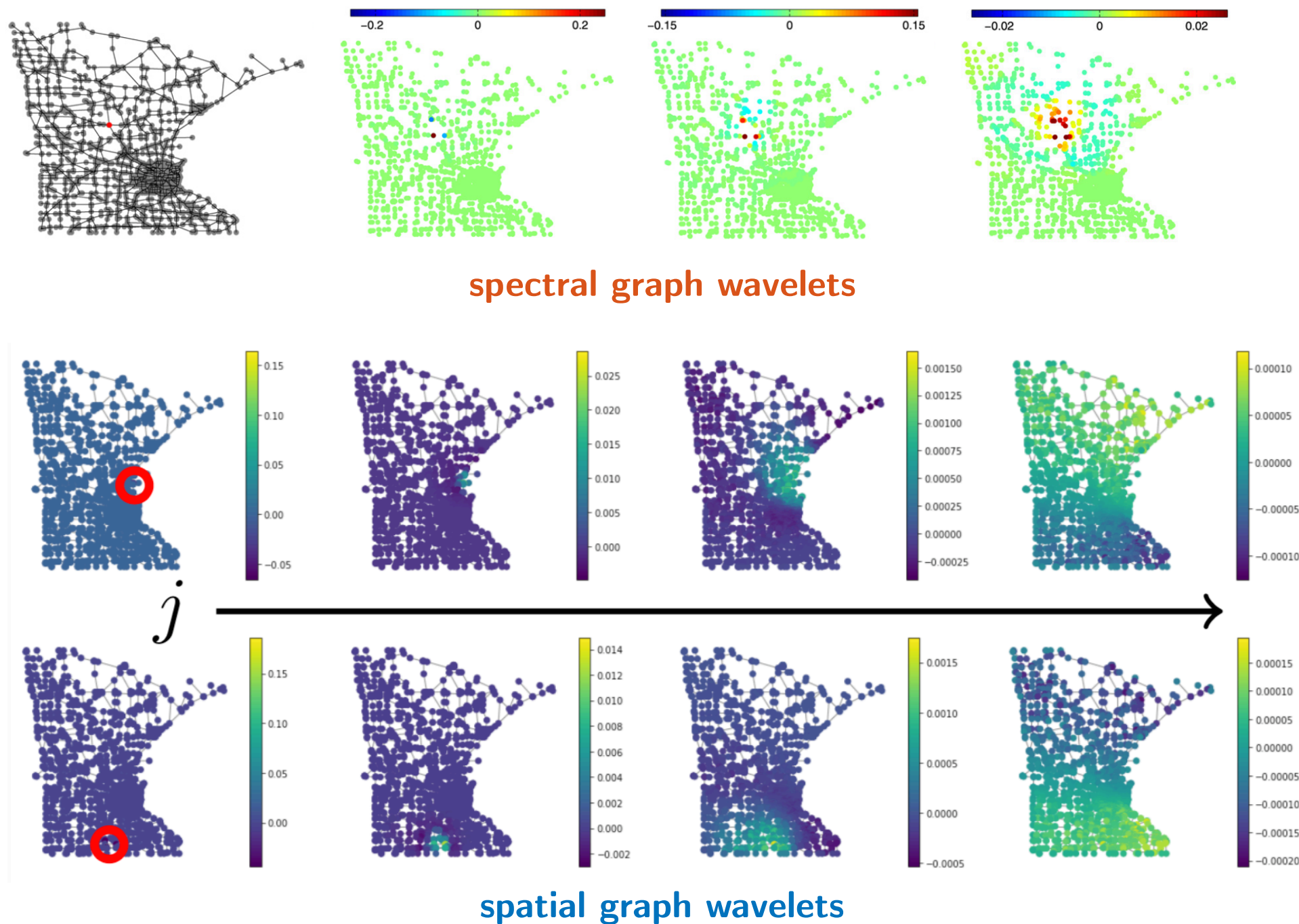
GSP for hierarchical modelling on graphs

Hierarchical modelling on graphs



- hierarchical modelling in GNNs
 - increase size of filter or number of layers
 - graph pooling (downsampling)
- multiscale transforms (e.g., wavelets) can be natural tools for this

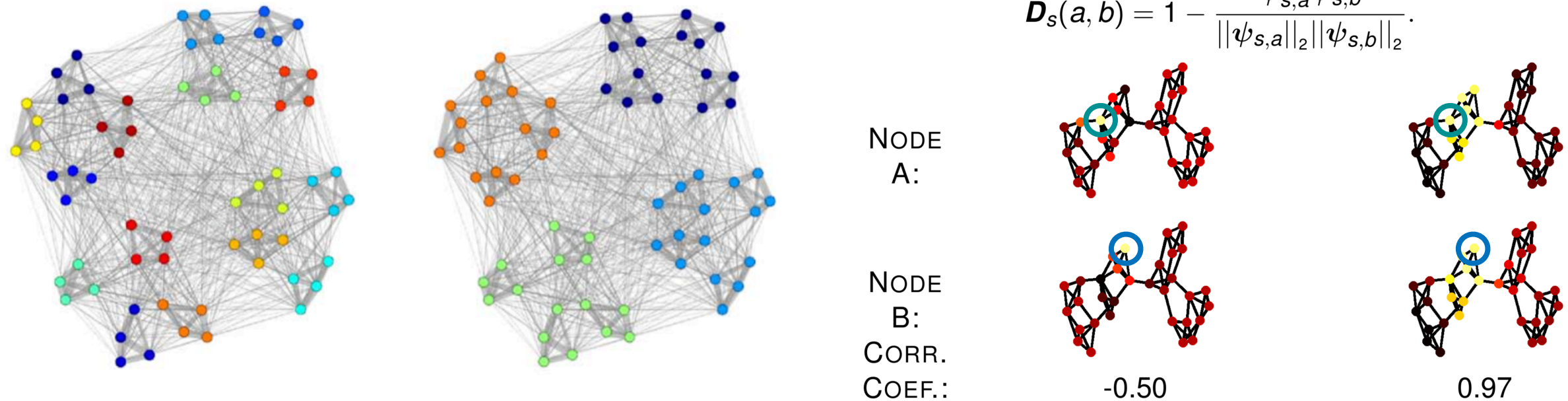
Wavelets on graphs



Hammond et al., "Wavelets on graphs via spectral graph theory," ACHA, 2011.

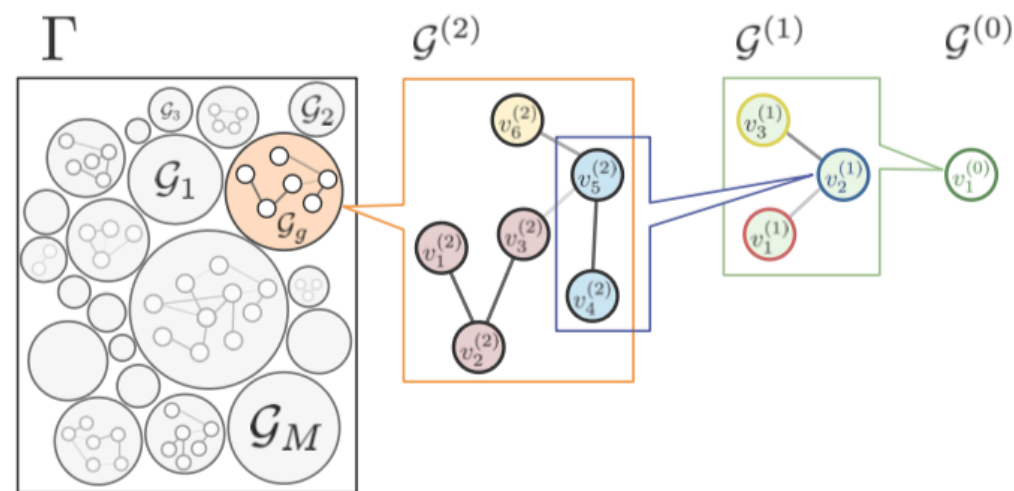
Gao et al., "Geometric scattering for graph data analysis," ICML, 2019.

Spectral graph wavelets for multiscale clustering

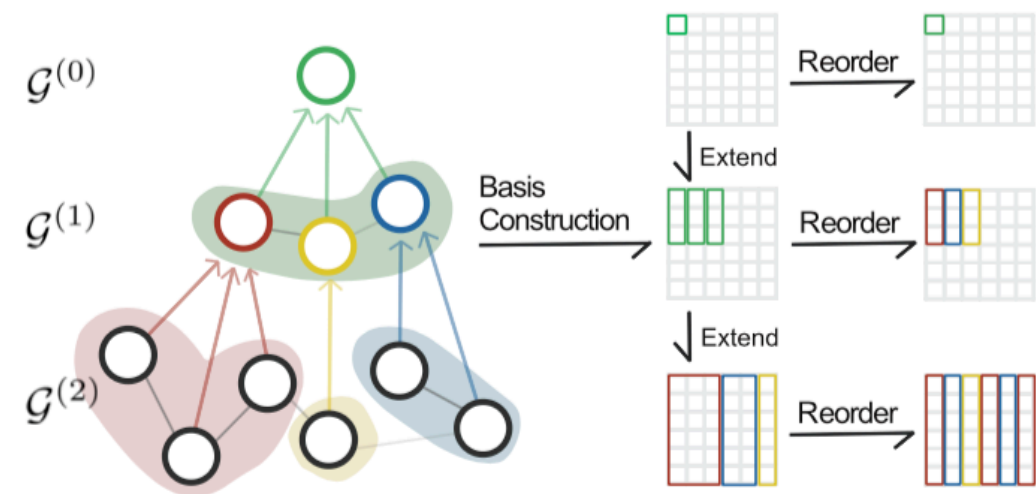


- spectral graph wavelets with different scales centred at node \mathbf{u} provides an “egocentered view” of the graph seen from \mathbf{u}
- similarity between nodes can be built at different levels to facilitate multiscale clustering

Haar-like wavelets for graph learning



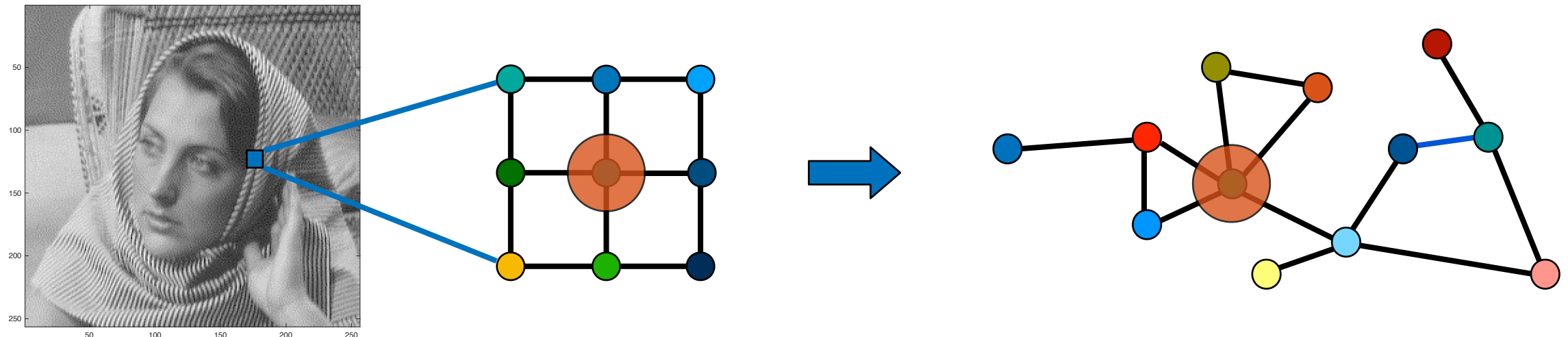
coarse-grained graph chain



orthogonal basis construction

- given a coarse-grained graph chain an orthogonal basis is constructed
- this can then be used for both graph convolution and hierarchical graph pooling

GSP for exploiting data structure - Summary



- GSP enables various definitions of convolution on graphs
- graph filters enrich design of convolutional learning models on graphs (both GNNs and graph-based GPs)
- multiscale transforms (in particular wavelets) facilitate hierarchical modelling on graphs

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