香港城市大學
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Decimated Framelet System on Graphs and Fast G-Framelet Transforms

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  - Wavelet-like systems on graphs
  - Orthogonal eigen-pairs and localized kernels
- **Framelets on Graphs and Fast G-Framelet Transforms (FGT)**
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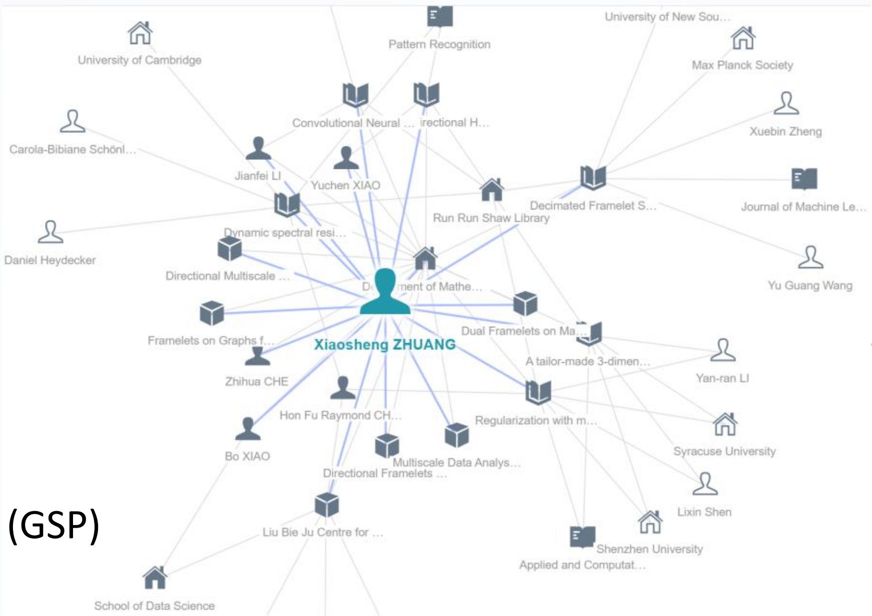
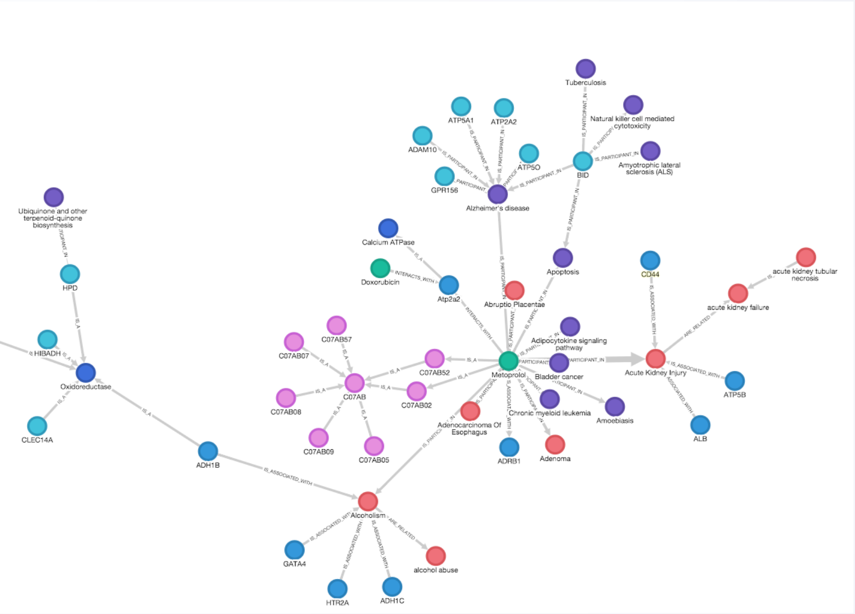
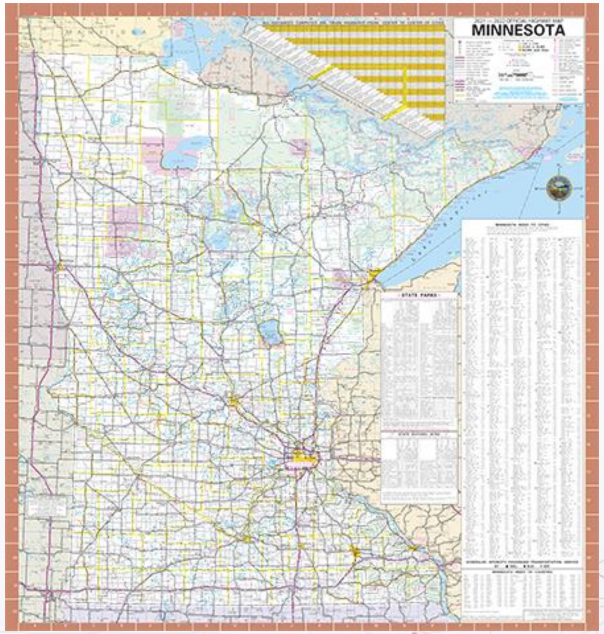
  - Filter Banks and Convolution
  - Multi-level G-framelet decomposition and reconstruction
- **GSP and GNNs via FGT**
  - Multiscale analysis
  - GNNs for graph classification

Introduction

- Graph Data
  - Social Networks
  - Road Networks
  - Drug interaction
- Graph Learning in
  - Graph signal processing (GSP)
  - Machine learning (ML)
  - Deep learning (DL)
  - Geometric deep learning (GDL)
  - Graph neural networks (GNNs)
- Tasks
  - Graph Clustering
  - Graph Classification







Introduction

- Graphs:

$$\mathcal{G} = (V, E, \boldsymbol{w})$$

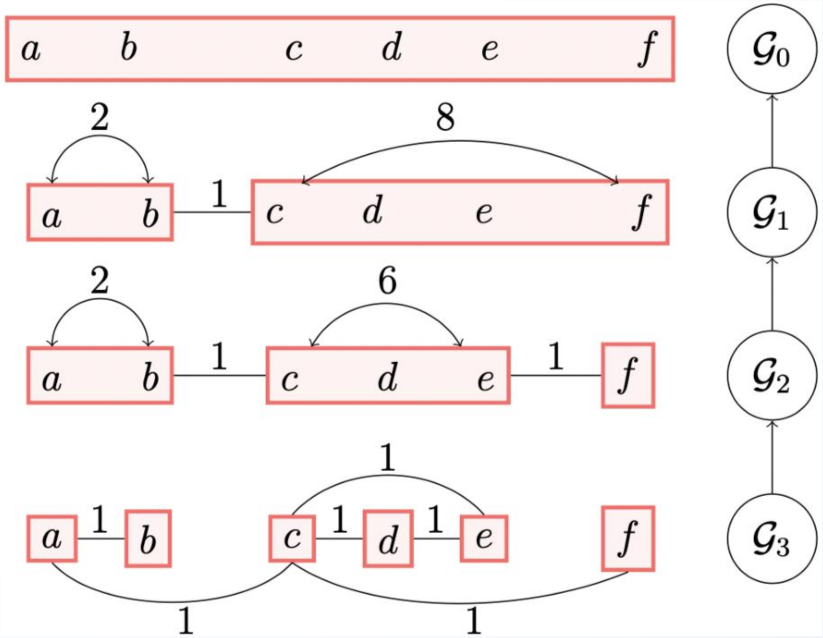
- Graph signals:

$$\boldsymbol{f} : V \to \mathbb{C}$$

- Graph (Hilbert) space:

$$l_2(\mathcal{G}) := l_2(\mathcal{G}, \langle \cdot, \cdot \rangle_{\mathcal{G}}) \quad \text{with} \quad \langle \boldsymbol{f}, \boldsymbol{g} \rangle_{\mathcal{G}} := \sum_{v \in V} \boldsymbol{f}(v)\overline{\boldsymbol{g}(v)}, \quad \boldsymbol{f}, \boldsymbol{g} \in l_2(\mathcal{G})$$

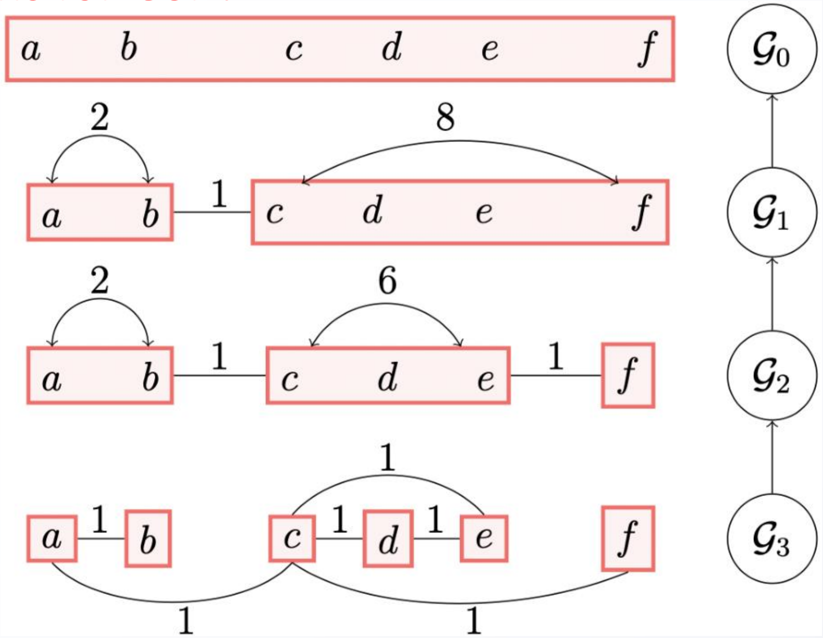
- Wavelet systems on **R**:
  - Dilations and translations of localized functions (wavelets)
  - Multiscale property and filter bank association (fast algorithms)
  - Excellent for Euclidean data (signals, images, videos, etc.)



- **Question**: How to construction wavelet-like systems on graphs for GSP?

Introduction

- **Question**: How to construction wavelet-like systems on graphs for GSP?
- **Answer**: via localized kernel on graph.



- Orthogonal eigen-pairs for $l_2(\mathcal{G})$ (e.g., from graph Laplacian)

$$\{(\boldsymbol{u}_\ell, \lambda_\ell)\}_{\ell=1}^N$$

- Localized kernel:

$$K_{j,\alpha}(p,v) := \sum_\ell \widehat{\alpha}\left(\frac{\lambda_\ell}{2^j}\right)\overline{\boldsymbol{u}_\ell(p)}\boldsymbol{u}_\ell(v), \text{ for } p, v \in V.$$

- Coarse-grained chain (multiscale through clustering)

$$\mathcal{G}_{J\to J_0} := (\mathcal{G}_J, \mathcal{G}_{J-1}, \ldots, \mathcal{G}_{J_0})$$

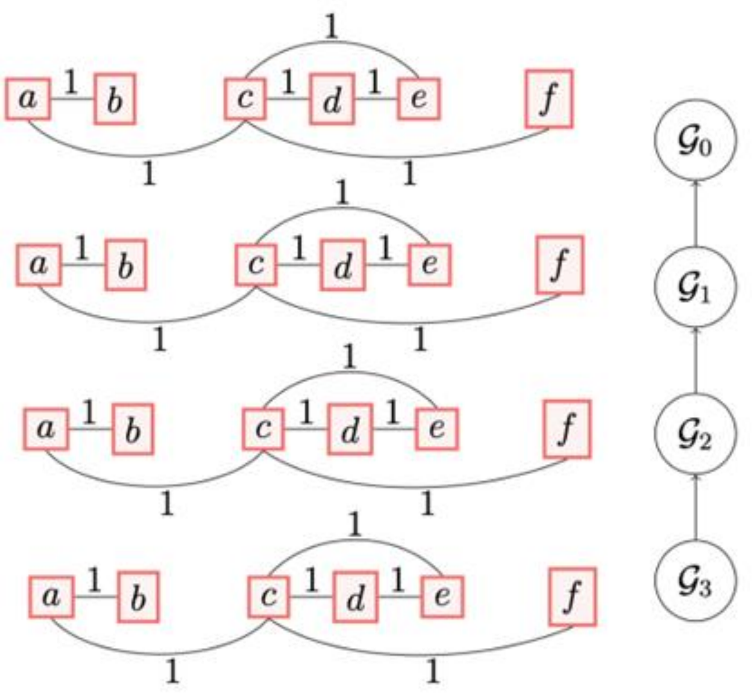
Framelets on Graphs (Undecimated Systems)

- Ingredients from R:
  - framelet system $\Psi_j = \{\alpha_j; \beta_j^{(1)}, \ldots, \beta_j^{(r_j)}\}$
  - filter bank $\boldsymbol{\eta}_j := \{a_j; b_j^{(1)}, \ldots, b_j^{(r_j-1)}\}$
  - refinement structure:

$$\widehat{\alpha_{j-1}}(\xi/\Lambda_{j-1}) = \widehat{a_j}(\xi/\Lambda_j)\widehat{\alpha_j}(\xi/\Lambda_j),$$
$$\widehat{\beta_{j-1}^{(n)}}(\xi/\Lambda_{j-1}) = \widehat{b_j^{(n)}}(\xi/\Lambda_j)\widehat{\alpha_j}(\xi/\Lambda_j), \quad n = 1, \ldots, r_{j-1}$$

- UFS (Undecimated framelet systems on graph, $\mathcal{G}_j \equiv \mathcal{G}$):

$$\boldsymbol{\varphi}_{j,p}(v) := \sum_{\ell=1}^{N} \widehat{\alpha}\left(\frac{\lambda_\ell}{2^j}\right)\overline{\boldsymbol{u}_\ell(p)}\boldsymbol{u}_\ell(v),$$
$$\boldsymbol{\psi}_{j,p}^{n}(v) := \sum_{\ell=1}^{N} \widehat{\beta^{(n)}}\left(\frac{\lambda_\ell}{2^j}\right)\overline{\boldsymbol{u}_\ell(p)}\boldsymbol{u}_\ell(v), \quad n = 1, \ldots, r.$$
$$\mathsf{UFS}_{J_1}^{J}(\Psi, \boldsymbol{\eta}) := \mathsf{UFS}_{J_1}^{J}(\Psi, \boldsymbol{\eta}; \mathcal{G})$$
$$:= \{\boldsymbol{\varphi}_{J_1,p} : p \in V\} \cup \{\boldsymbol{\psi}_{j,p}^{n} : p \in V, n = 1, \ldots, r, j = J_1, \ldots, J\}$$



Framelets on Graphs (Decimated Systems)

- Ingredients from R:
  - framelet system $\Psi_j = \{\alpha_j; \beta_j^{(1)}, \ldots, \beta_j^{(r_j)}\}$
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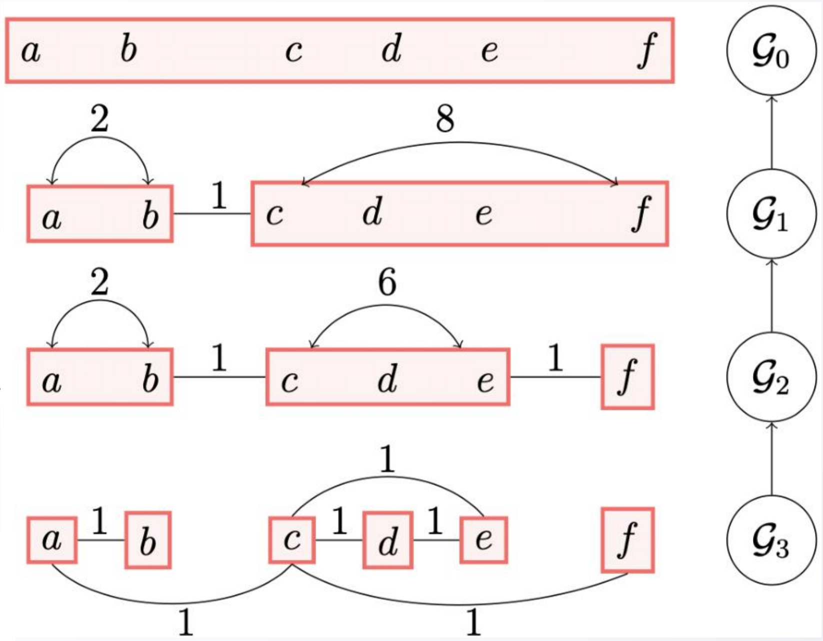


- DFS (Decimated framelet systems on graph, $\mathcal{G}_j$ different):

$$\boldsymbol{\varphi}_{j,[p]}(v) := \sqrt{\omega_{j,[p]}} \sum_{\ell=1}^{N} \widehat{\alpha_j}\left(\frac{\lambda_\ell}{\Lambda_j}\right) \overline{\boldsymbol{u}_\ell([p])} \boldsymbol{u}_\ell(v), \quad [p] \in V_j,$$

$$\boldsymbol{\psi}_{j,[p]}^n(v) := \sqrt{\omega_{j+1,[p]}} \sum_{\ell=1}^{N} \widehat{\beta_j^{(n)}}\left(\frac{\lambda_\ell}{\Lambda_j}\right) \overline{\boldsymbol{u}_\ell([p])} \boldsymbol{u}_\ell(v), \quad [p] \in V_{j+1},\ n = 1, \ldots, r_j$$

$$\mathrm{DFS}(\{\Psi_j\}_{j=J_1}^{J}, \{\boldsymbol{\eta}_j\}_{j=J_1+1}^{J}) := \{\boldsymbol{\varphi}_{J_1,[p]} : [p] \in V_{J_1}\} \cup \{\boldsymbol{\psi}_{j,[p]}^n : [p] \in V_{j+1},\ j = J_1, \ldots, J\}.$$

Framelets on Graphs

- Characterization Theorems for decimated **Tight** framelet system:

$$\|\boldsymbol{f}\|^2 = \sum_{[p]\in V_{J_1}} \left|\left\langle \boldsymbol{f}, \varphi_{J_1,[p]} \right\rangle\right|^2 + \sum_{j=J_1}^{J} \sum_{n=1}^{r_j} \sum_{[p]\in V_{j+1}} \left|\left\langle \boldsymbol{f}, \psi^{n}_{j,[p]} \right\rangle\right|^2 \quad \forall \boldsymbol{f} \in l_2(\mathcal{G}),\ J_1 = J_0, \ldots, J.$$

  - In terms of $\Psi_j = \{\alpha_j; \beta_j^{(1)}, \ldots, \beta_j^{(r_j)}\}$

$$1 = \left|\widehat{\alpha_J}\left(\frac{\lambda_\ell}{\Lambda_J}\right)\right|^2 + \sum_{n=1}^{r_J} \left|\widehat{\beta_J^{(n)}}\left(\frac{\lambda_\ell}{\Lambda_J}\right)\right|^2,$$

$$\overline{\widehat{\alpha_{j+1}}\left(\frac{\lambda_\ell}{\Lambda_{j+1}}\right)} \widehat{\alpha_{j+1}}\left(\frac{\lambda_{\ell'}}{\Lambda_{j+1}}\right) \mathcal{U}_{\ell,\ell'}(\mathcal{Q}_{j+1}) - \overline{\widehat{\alpha_j}\left(\frac{\lambda_\ell}{\Lambda_j}\right)} \widehat{\alpha_j}\left(\frac{\lambda_{\ell'}}{\Lambda_j}\right) \mathcal{U}_{\ell,\ell'}(\mathcal{Q}_j)$$

$$= \sum_{n=1}^{r_j} \overline{\widehat{\beta_j^{(n)}}\left(\frac{\lambda_\ell}{\Lambda_j}\right)} \widehat{\beta_j^{(n)}}\left(\frac{\lambda_{\ell'}}{\Lambda_j}\right) \mathcal{U}_{\ell,\ell'}(\mathcal{Q}_{j+1}) \quad \forall j = J_0, \ldots, J-1, \quad \mathcal{U}_{\ell,\ell'}(\mathcal{Q}_j) := \sum_{[p]\in V_j} \omega_{j,[p]}\, \boldsymbol{u}_\ell([p]) \overline{\boldsymbol{u}_{\ell'}([p])}$$

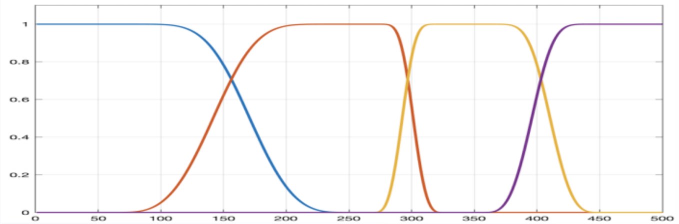
  - In terms of filter bank $\boldsymbol{\eta}_j := \{a_j; b_j^{(1)}, \ldots, b_j^{(r_j-1)}\}$

$$\overline{\widehat{a_j}\left(\frac{\lambda_\ell}{\Lambda_j}\right)} \widehat{a_j}\left(\frac{\lambda_{\ell'}}{\Lambda_j}\right) \mathcal{U}_{\ell,\ell'}(\mathcal{Q}_{j-1}) + \sum_{n=1}^{r_j-1} \overline{\widehat{b_j^{(n)}}\left(\frac{\lambda_\ell}{\Lambda_j}\right)} \widehat{b_j^{(n)}}\left(\frac{\lambda_{\ell'}}{\Lambda_j}\right) \mathcal{U}_{\ell,\ell'}(\mathcal{Q}_j) = \mathcal{U}_{\ell,\ell'}(\mathcal{Q}_j)$$

- Construction:
  - Graph clustering algorithms for the coarse-grained chain (multi-scale)
  - Orthogonal eigen-pairs through graph Laplacian and Gram-Schmidt orthogonalization
  - Careful design of filter banks so that $\mathcal{U}_{\ell,\ell'}(\mathcal{Q}_j) = \delta_{\ell,\ell'}$

Fast G-Framelet Transforms (FGT)

- Ingredients:
  - PR filter banks



$$\left|\widehat{a_j}\left(\frac{\lambda_\ell}{\Lambda_j}\right)\right|^2 + \sum_{n=1}^{r_j-1}\left|\widehat{b_j^{(n)}}\left(\frac{\lambda_\ell}{\Lambda_j}\right)\right|^2 = 1$$

  - Discrete Fourier transforms (DFT and adjoint DFT) on graphs:

$$(\mathbf{F}_j^*\mathbf{v})_\ell := \sum_{[p]\in V_j} \mathbf{v}([p])\,\sqrt{\omega_{j,[p]}}\,\overline{\boldsymbol{u}_\ell([p])}, \quad \ell\in\Omega_j.$$

$$[\mathbf{F}_j\boldsymbol{c}]([p]) := \sum_{\ell\in\Omega_j} c_\ell\,\sqrt{\omega_{j,[p]}}\,\boldsymbol{u}_\ell([p]), \quad [p]\in V_j,\ \boldsymbol{c}=(c_\ell)_{\ell=1}^{N_j}\in l_2(\Omega_j).$$

  - Discrete convolution, down- and up-sampling operators on graphs

$$[\mathbf{v} *_j h]([p]) := \sum_{\ell\in\Omega_j} \widehat{\mathrm{v}}_\ell\,\widehat{h}\left(\frac{\lambda_\ell}{\lambda_{N_j}}\right)\sqrt{\omega_{j,[p]}}\,\boldsymbol{u}_\ell([p]), \quad [p]\in V_j$$

$$[\mathbf{v}{\downarrow_j}]([p]) := \sum_{\lambda_\ell\in\Omega_{j-1}} \widehat{\mathrm{v}}_\ell\,\sqrt{\omega_{j-1,[p]}}\,\boldsymbol{u}_\ell([p]), \quad [p]\in V_{j-1}$$

$$[\mathbf{v}{\uparrow_j}]([p]) := \sum_{\ell\in\Omega_{j-1}} \widehat{\mathrm{v}}_\ell\sqrt{\omega_{j,[p]}}\,\boldsymbol{u}_\ell([p]), \quad [p]\in V_j$$

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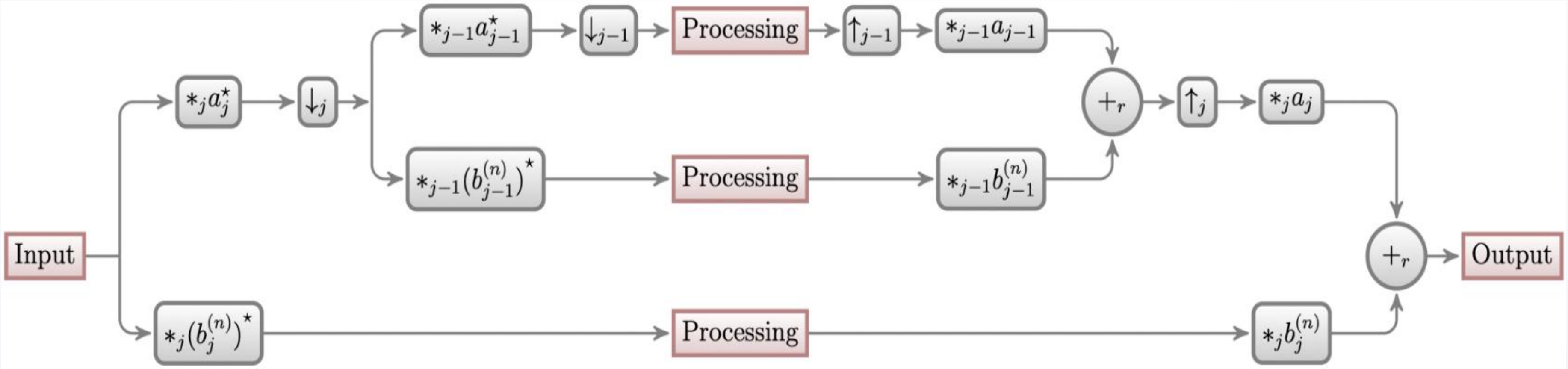
Fast G-Framelet Transforms (FGT)

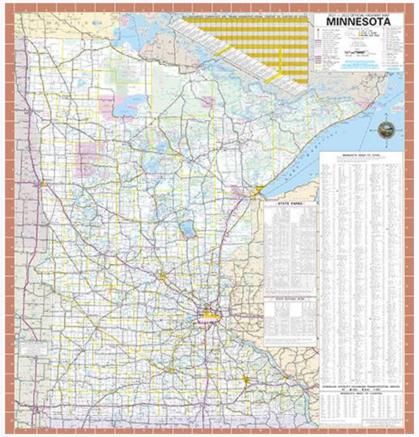
- Ingredients:
  - PR filter banks
  - Discrete Fourier transforms (DFT and adjoint DFT) on graphs
  - Discrete convolution, down- and up-sampling operators on graphs

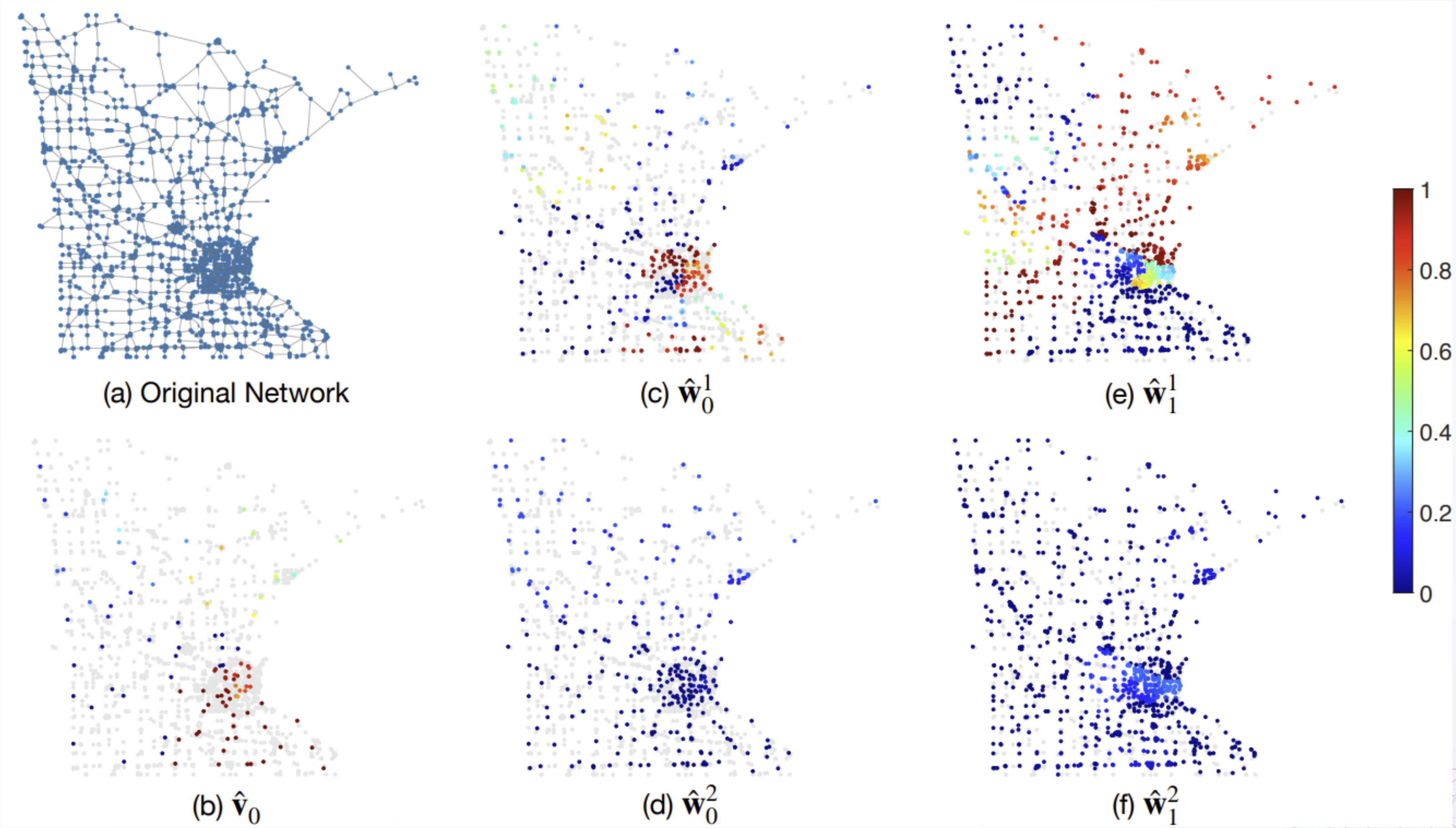
- Multilevel G-framelet decomposition and reconstruction (**FGT**):



Graph Signal Representation via FGT

- <u>Multiscale Representation</u>





GNNs via FGT

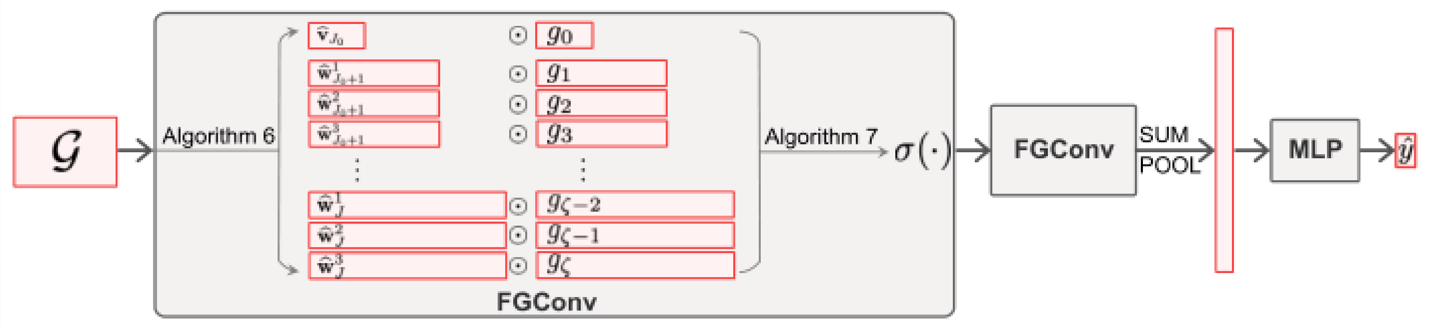
- FGConv (framelet graph convolution):

$$g \star f = \mathbf{V}\big((\mathbf{W}g) \odot (\mathbf{W}f)\big)$$

  - ***g***: trained filter
  - ***f***: graph signal.
  - **V**, **W**: FGT decomposition and reconstruction operators

$$\mathcal{F}^{\mathrm{out}} = \sigma\big(\mathbf{V}(G(\mathbf{W}(\mathcal{F}^{\mathrm{in}}\mathcal{W})))\big).$$

- GNN architecture via FGConv:



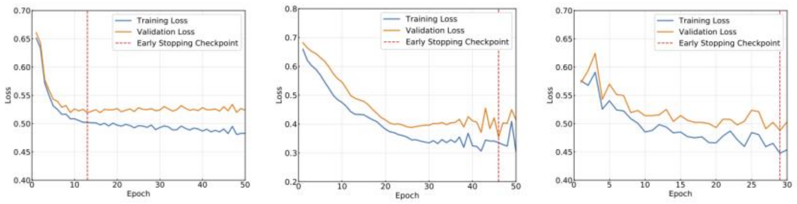
FGConv – FGConv – SumPool – MLP.

GNNs via FGT

- Graph Data Sets and Classification

Table 4: Statistical information of the datasets used for graph classification

Datasets	PROTEINS	MUTAG	D&D
Max. #Nodes	620	28	5,748
Min. #Nodes	4	10	30
Avg. #Nodes	39.06	17.93	284.32
Avg. #Edges	72.82	19.79	715.66
#Graphs	1,113	188	1,178
#Classes	2	2	2



(a) PROTEINS (b) MUTAG (c) D&D

Figure 9: Plots of losses against epoch from one repetition on the three benchmark graph classification datasets. The early stopping chechpoint corresponds to the epoch where the model is saved for evaluation on the test set, i.e. when the smallest validation loss was achieved.

Table 5: Mean test accuracy (in percentage) and standard deviation of FGConv-Sum as compared with existing methods on the benchmark graph classification datasets, over 10 repetitions.

Methods	PROTEINS	MUTAG	D&D
SP	75.07*	85.79*	–
Graphlet	71.67*	81.58*	78.45*
RW	74.22*	83.68*	–
WL	72.92*	80.72*	77.95*
GIN	76.2	**89.4**	–
PatchySan	75.00	**91.58**	76.27
DGCNN	75.54	85.83	79.37
DiffPool	76.25	–	**80.64**
SAGPool	72.17	–	77.07
EigenPool	**76.6**	–	78.6
g-U-Nets	**77.68**	–	**82.43**
FGConv-Sum	**78.3±2.26**	**90.8±2.50**	**82.9±2.55**

'*' denotes the record retrieved from Niepert et al. (2016).
'–' means that there is no public record for the method on the dataset.
! The records without superscription are retrieved from their corresponding original papers.
! The decimal place is not modified when transferring the results.
! The top three scores are highlighted as: **First**, **Second**, and **Third**.

Summary

- Graph signal processing (GSP), machine learning (ML), deep learning (DL), geometric deep learning (GDL), and graph neural networks (GNNs) deal with common graph structure data.
- Wavelet-like systems on graphs play an important role in the above areas like the wavelet/framelet systems on Euclidean spaces.
- In terms of the localized kernel method for defining “dilation” and “translation”, we can construct decimated and undecimated framelets on graphs based on coarse-grained chains and orthogonal eigen-pairs.
- Fast G-framelet transforms (FGT) are established with filter bank association
- Applications of FGT in graph signal representation (Minnesota road network) are presented.
- FGT can be used to define graph convolution (FGConv) for graph neural networks (GNNs). We build a GNN with the FGConv-FGConv-SumPool-MLP architecture.
- Applications of our GNNs in graph classification demonstrate state-of-the-art performance.

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