

# Bridging graph signal processing and graph neural networks

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# Graph-structured data

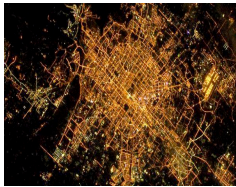
## Data with explicit graph



Social  
networks



Internet of  
things

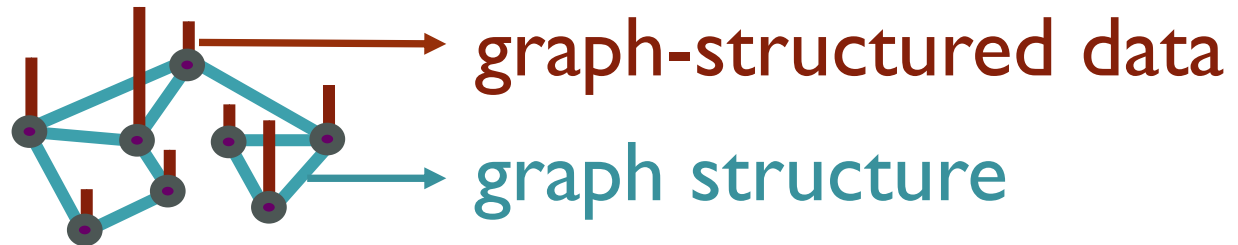


Traffic  
networks



Human brain  
networks

# Graph-structured data



## Data with explicit graph



Social  
networks



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things

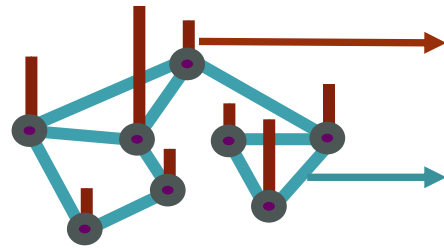


Traffic  
networks



Human brain  
networks

# Graph-structured data



graph-structured data

graph structure

Data with explicit graph



Social networks



Internet of things

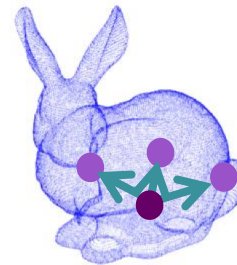


Traffic networks



Human brain networks

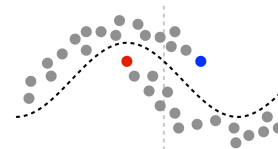
Data with implicit graph



3D point cloud



Action recognition



Semi-supervised learning

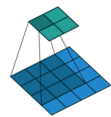
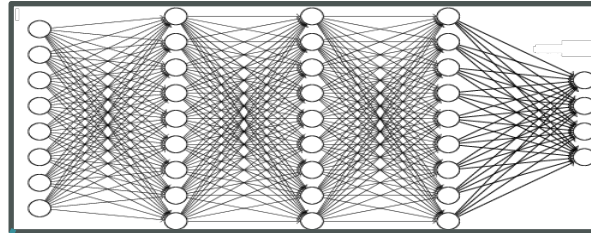


Recommender systems

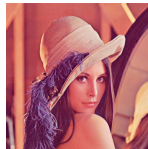
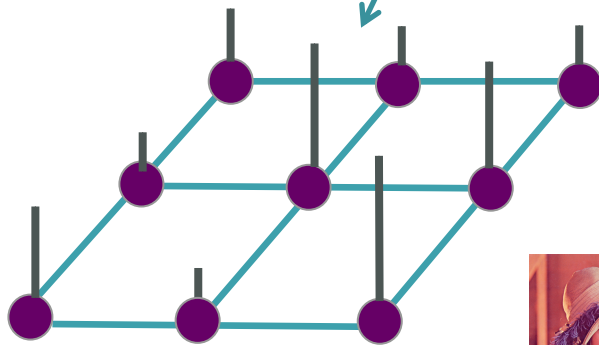


# Graph-structured data

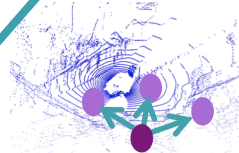
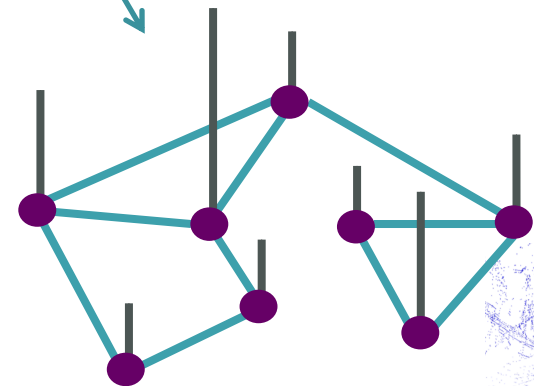
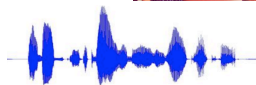
Data science toolbox



Convolution



data associated with  
**regular** graphs



data associated with  
**irregular** graphs



# Graph-structured data science

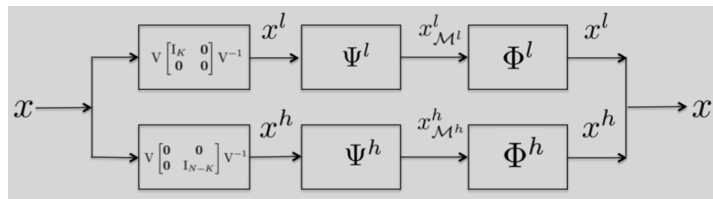
A data-science toolbox to process and learn from data associated with large-scale, complex, irregular graphs

# Graph-structured data science

A data-science toolbox to process and learn from data associated with large-scale, complex, irregular graphs

## Graph signal processing (GSP)

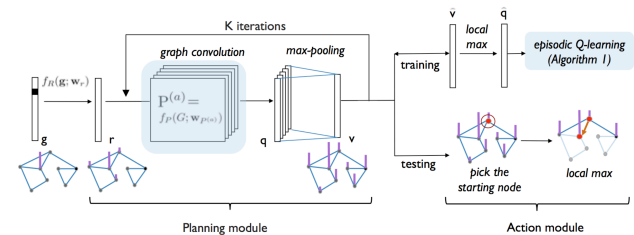
- Extend classical signal processing
- Analytical model
- Theoretical guarantee



Graph filter bank

## Graph neural network (GNN)

- Extend deep learning techniques
- Data-driven model
- Empirical performance



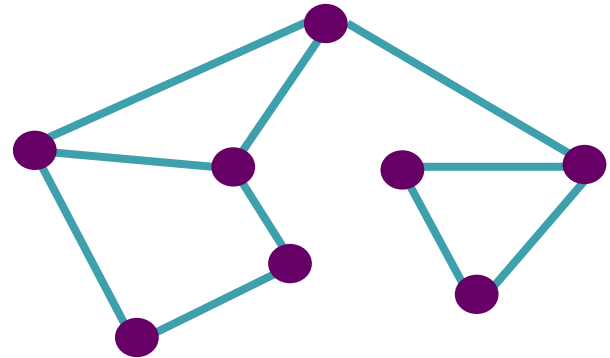
Graph neural network

# Sampling & recovery of graph-structured data

# GSP: Sampling & recovery

**Task:** Approximate the original graph-structured data by exploiting information from its subset

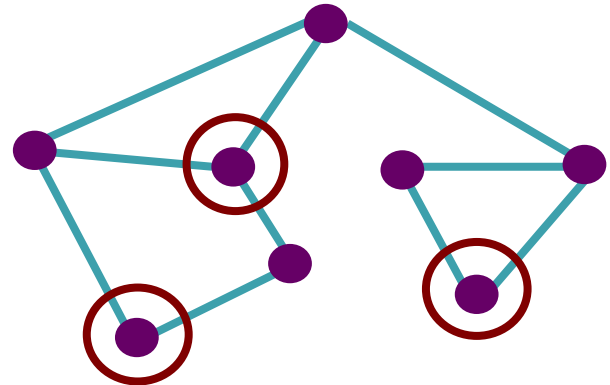
Look for data at each node



# GSP: Sampling & recovery

**Task:** Approximate the original graph-structured data by exploiting information from its subset

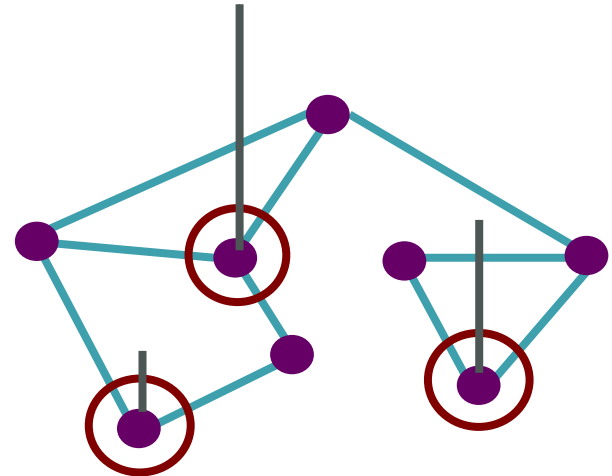
Select a few representative nodes



# GSP: Sampling & recovery

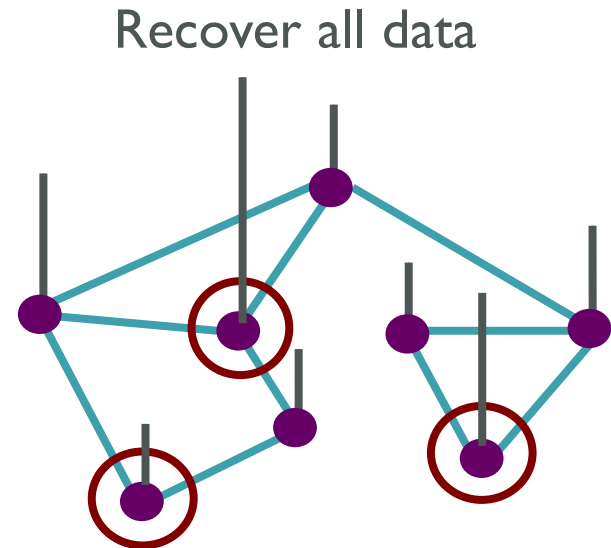
**Task:** Approximate the original graph-structured data by exploiting information from its subset

Query values at selected nodes



# GSP: Sampling & recovery

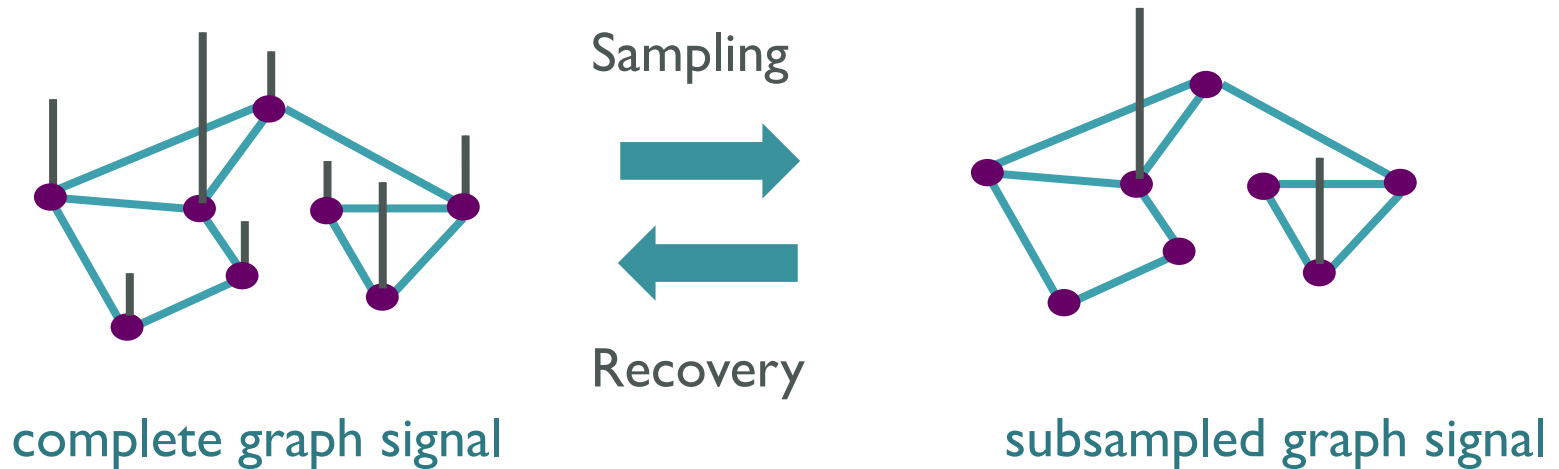
**Task:** Approximate the original graph-structured data by exploiting information from its subset





# GSP: Sampling & recovery

**Task:** Approximate the original graph-structured data by exploiting information from its subset

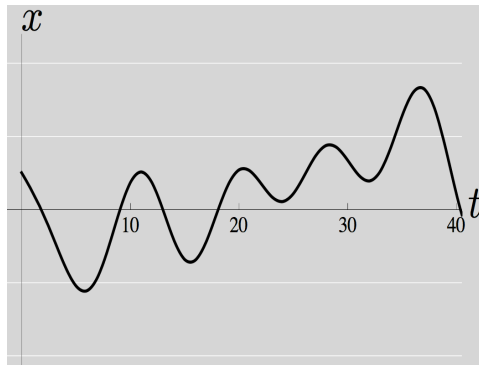


$$\text{sampling :} \quad \mathbf{x}' = \Psi \mathbf{x}$$

$$\text{recovery :} \quad \mathbf{x} = \Phi \mathbf{x}'$$

# GSP: Sampling & recovery

**Task:** Approximate the original graph-structured data by exploiting information from its subset

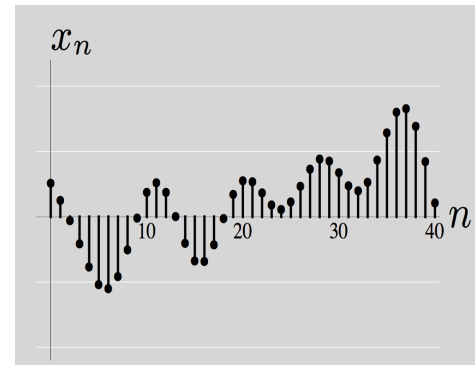


complete continuous signal

Sampling



Recovery

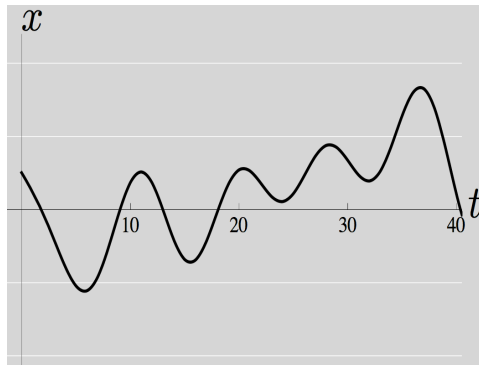


subsampled sequence



# GSP: Sampling & recovery

**Task:** Approximate the original graph-structured data by exploiting information from its subset

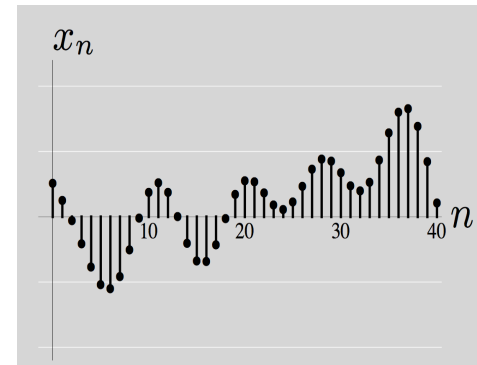


complete continuous signal

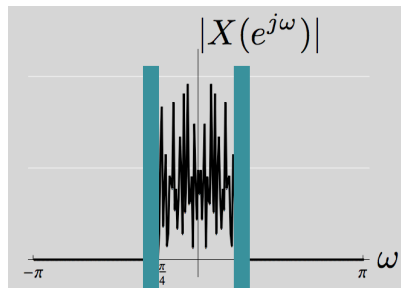
Sampling



Recovery



subsampled sequence

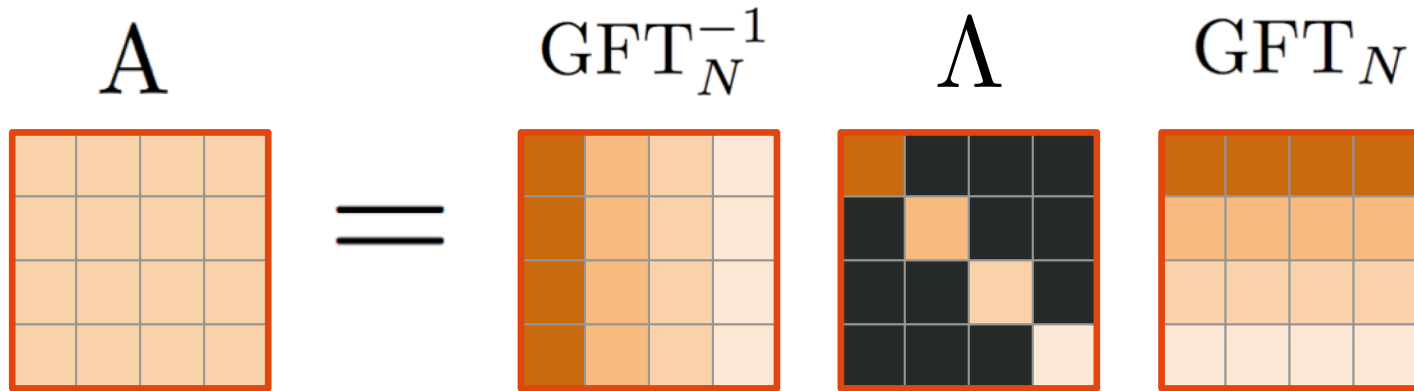


**bandlimited** in the Fourier domain



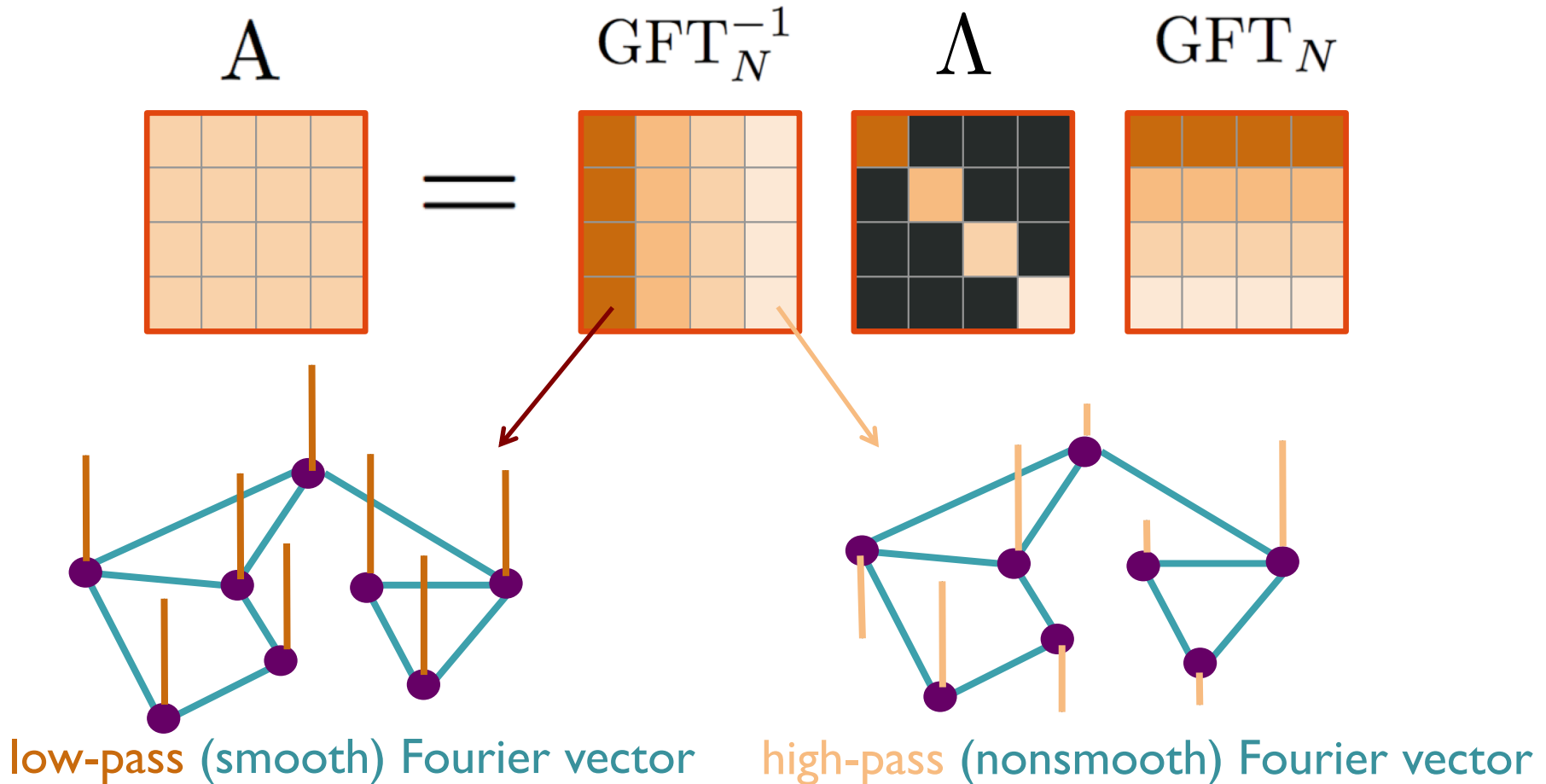
# GSP: Sampling & recovery

Graph Fourier transform

$$\mathbf{A} = \mathbf{GFT}_N^{-1} \mathbf{\Lambda} \mathbf{GFT}_N$$


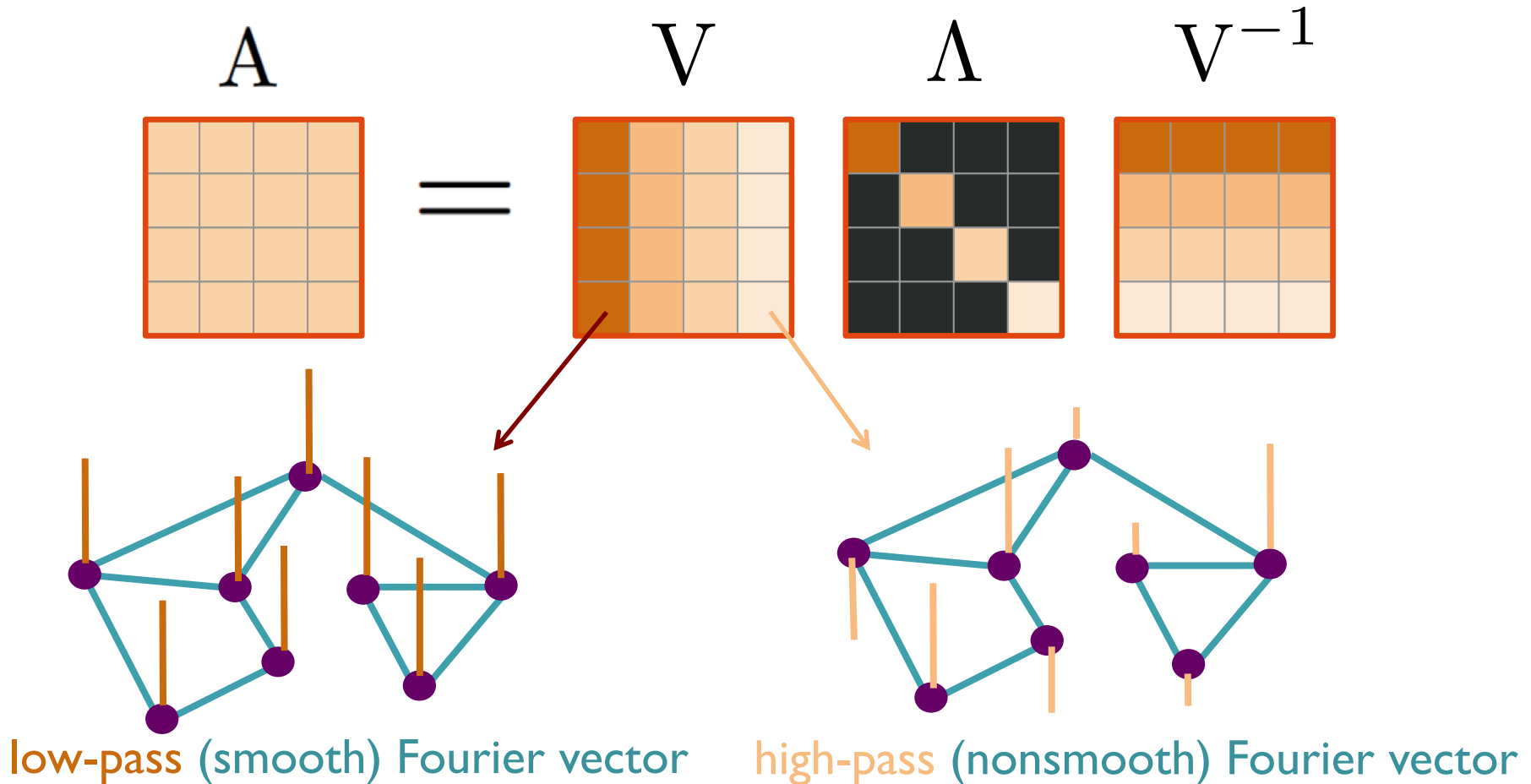
# GSP: Sampling & recovery

Graph Fourier transform



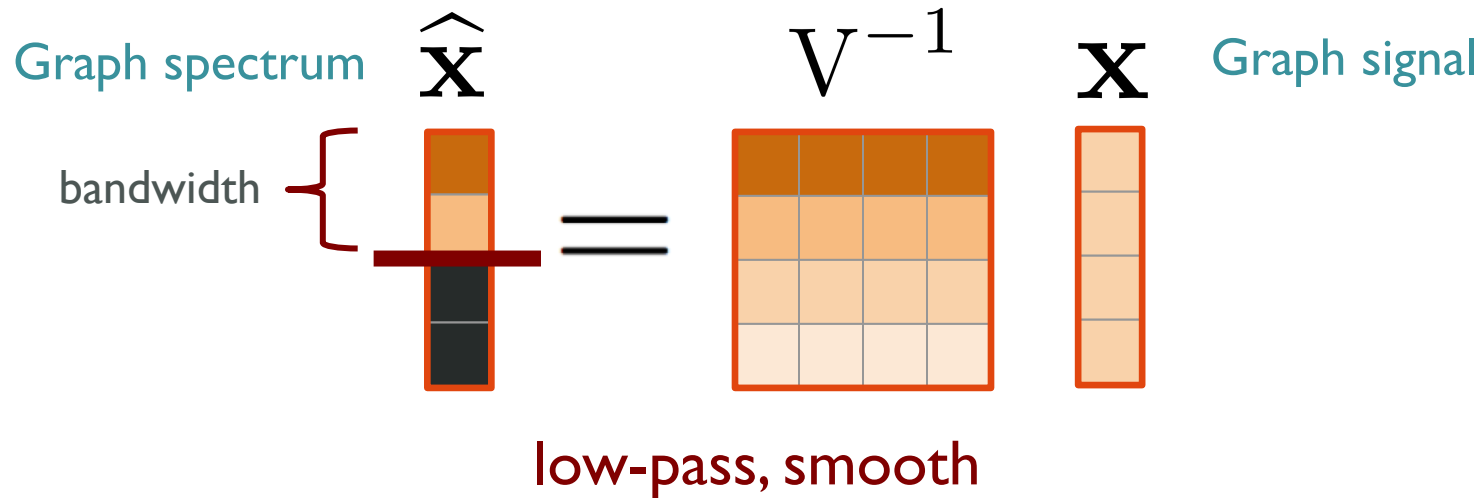
# GSP: Sampling & recovery

Graph Fourier transform



# GSP: Sampling & recovery

Bandlimited graph signals

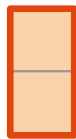


# GSP: Sampling & recovery

## Problem formulation

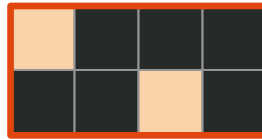
- Sampling process

$\mathbf{x}'$



=

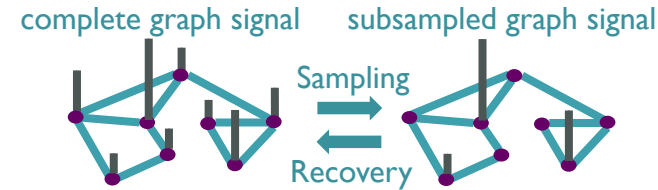
$\Psi$



$\mathbf{x}$



graph signal:  
bandlimited class



- Recovery process

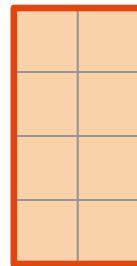
reconstruction

$\mathbf{x}$



=

$\Phi$



$\mathbf{x}'$

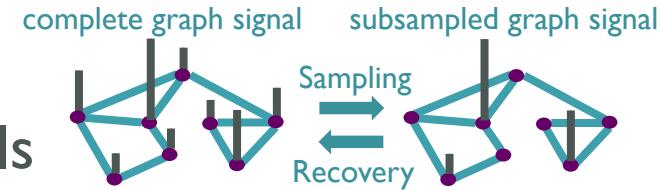


subsamples



# GSP: Sampling & recovery

Perfect recovery of bandlimited graph signals



**Theorem 1.** Let  $\Psi$  satisfy **qualified sampling operator**

$$\text{rank}(\Psi V_{(K)}) = K,$$

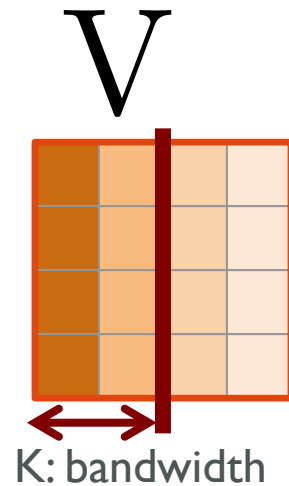
where  $V_{(K)} \in \mathbb{R}^{N \times K}$  denotes the first  $K$  columns of  $V$ . For all  $x \in \text{BL}_K(V^{-1})$ , perfect recovery,  $x = \Phi \Psi x$ , is achieved by choosing

$$\Phi = V_{(K)} U,$$

with  $U \Psi V_{(K)}$  a  $K \times K$  identity matrix.

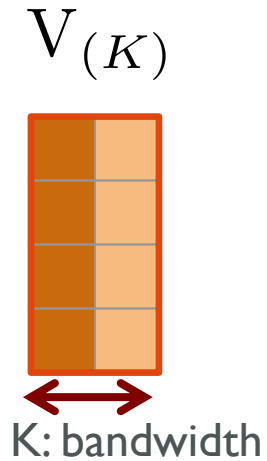
# GSP: Sampling & recovery

Sufficient condition for a qualified sampling operator



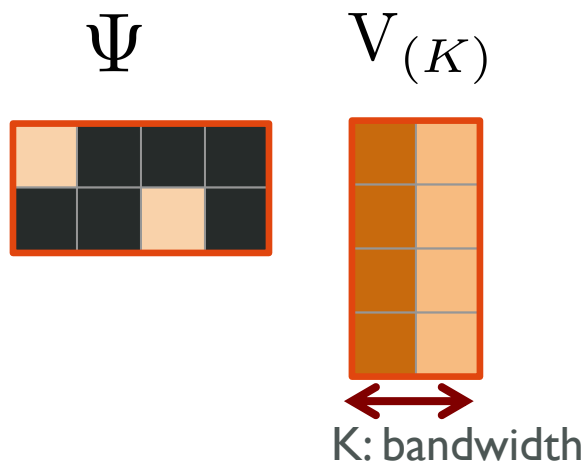
# GSP: Sampling & recovery

Sufficient condition for a qualified sampling operator



# GSP: Sampling & recovery

Sufficient condition for a qualified sampling operator

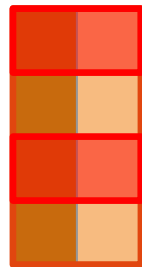
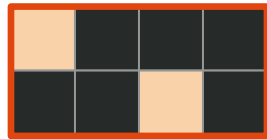


# GSP: Sampling & recovery

Sufficient condition for a qualified sampling operator

full rank: linearly independent

$$\Psi \quad V_{(K)}$$



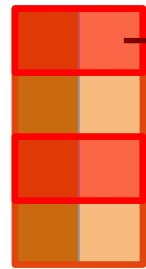
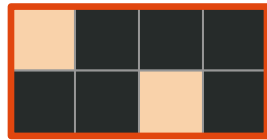
K: bandwidth

# GSP: Sampling & recovery

Sufficient condition for a qualified sampling operator

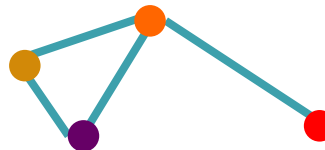
full rank: linearly independent

$$\Psi \quad V_{(K)}$$

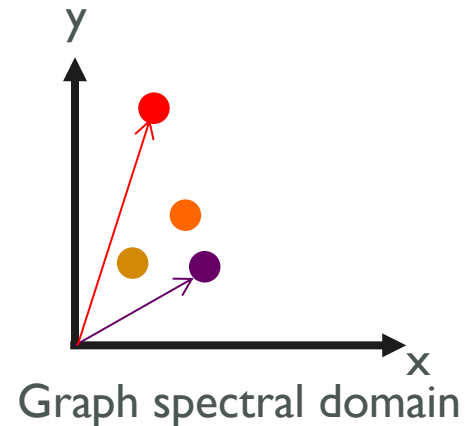


$\longleftrightarrow$   
K: bandwidth

node features/coordinates in the  
graph spectral domain



Graph vertex domain



Graph spectral domain

# GSP: Sampling & recovery

Sufficient condition for a qualified sampling operator

- Full rank  $\text{rank}(\Psi V_{(K)}) = K$

Optimal sampling operator

- Robust to noise
- Greedy algorithm

$$\mathbf{x}_{\mathcal{M}} = \Psi \mathbf{x} + \mathbf{e}$$

$\|\mathbf{e}\|_2 = C$

$$\begin{aligned} \Psi^{\text{opt}} &= \arg \min_{\Psi} \max_{\mathbf{x}} \|\Phi(\Psi \mathbf{x} + \mathbf{e}) - \mathbf{x}\|_2 \\ &= \arg \min_{\Psi} \left\| (\Psi V_{(K)})^{\dagger} \right\|_2 \end{aligned}$$

---

**Algorithm 1** Optimal Sampling Operator via Greedy Algorithm

---

**Input**  $V_{(K)}$  the first  $K$  columns of  $V$   
 $M$  the number of samples  
**Output**  $\mathcal{M}$  sampling set  
**Function**

```

while  $|\mathcal{M}| < M$ 
   $m = \arg \max_i \sigma_{\min}((V_{(K)})_{\mathcal{M}+\{i\}})$ 
   $\mathcal{M} \leftarrow \mathcal{M} + \{m\}$ 
end
return  $\mathcal{M}$ 

```

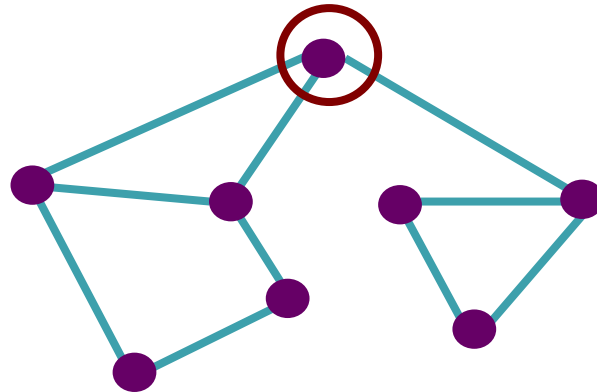
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# GSP: Sampling & recovery

## Sampling process

- Deterministic: Either choose a node or discard; Accurate
- Randomized: Sample nodes according to a distribution; fast, scalable
  - Fundamental limits of sampling ability

sampling probability  $\pi_i$





# GSP: Sampling & recovery

Fundamental limits of sampling strategies  $|\mathcal{M}| = m \rightarrow \infty$

- Minmax recovery error

$$\inf_{(\mathbf{x}^*, \mathcal{M}) \in \Theta_{\text{exp}}} \sup_{\mathbf{x} \in \text{ABL}_A(K, \beta, \mu)} \mathbb{E}_{\mathcal{M}} \left( \frac{\|\mathbf{x}^* - \mathbf{x}\|_2^2}{\|\mathbf{x}\|_2^2} \right)$$

$\downarrow$   
Sampling strategy

Reconstruction error

# GSP: Sampling & recovery

Fundamental limits of sampling strategies  $|\mathcal{M}| = m \rightarrow \infty$

- Minmax recovery error

$$\text{lower bound} \quad cm^{-\gamma_1} \leq \inf_{(\mathbf{x}^*, \mathcal{M}) \in \Theta_{\text{exp}}} \sup_{\mathbf{x} \in \text{ABL}_A(K, \beta, \mu)} \mathbb{E}_{\mathcal{M}} \left( \frac{\|\mathbf{x}^* - \mathbf{x}\|_2^2}{\|\mathbf{x}\|_2^2} \right) \leq Cm^{-\gamma_2} \quad \text{upper bound}$$

$$\boxed{\gamma_1 = \gamma_2}$$

Tight bound

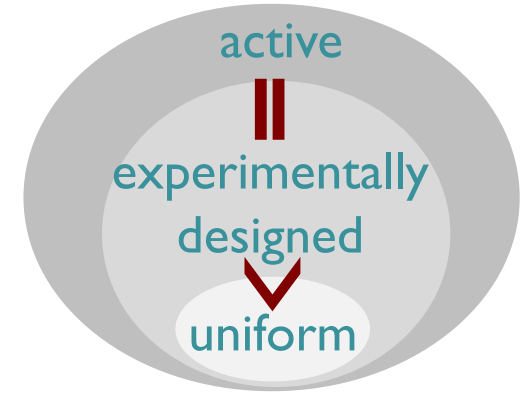
- Lower bound: fundamental limits
- Upper bound: optimal algorithm

higher rate  $\Rightarrow$  faster decay  $\Rightarrow$  better sampling

# GSP: Sampling & recovery

## Sampling process

- Fundamental limits of sampling strategies
  - Minmax recovery error
  - Lower bound
  - Sampling algorithm
  - Upper bound



**Corollary 6.** Let  $A \in \mathbb{R}^{N \times N}$  be a type-2 graph with parameter  $\kappa$ , for the class  $\mathcal{A}(K, \beta, \mu)$ .

## Uniform sampling

- Under uniform sampling,

$$cm^{-\frac{2\beta}{2\beta+\gamma}} \leq$$

$$\gamma_1 = \gamma_2 = \frac{2\beta}{2\beta+\gamma}, \quad \gamma > 1$$

where constant  $C > c > 0$ , and the rate is achieved when  $\kappa$  is in the order of  $m^{1/(2\beta+\gamma)}$  and  $\gamma = \log(N)/\log(\kappa) \geq 1$ ;

## Experimentally designed sampling & feedback-based sampling

$$cm^{-\frac{2\beta}{2\beta+1}} \leq$$

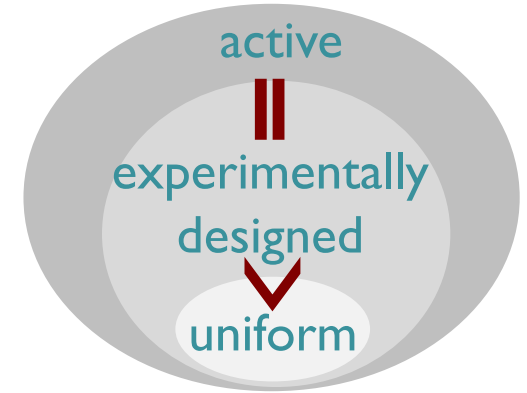
$$\gamma_1 = \gamma_2 = \frac{2\beta}{2\beta+1}$$

where constant  $C > 0$ , the rate is achieved when  $\kappa$  is in the order of  $m^{1/(2\beta+1)}$  and upper bounded by  $N$ .

# GSP: Sampling & recovery

## Sampling process

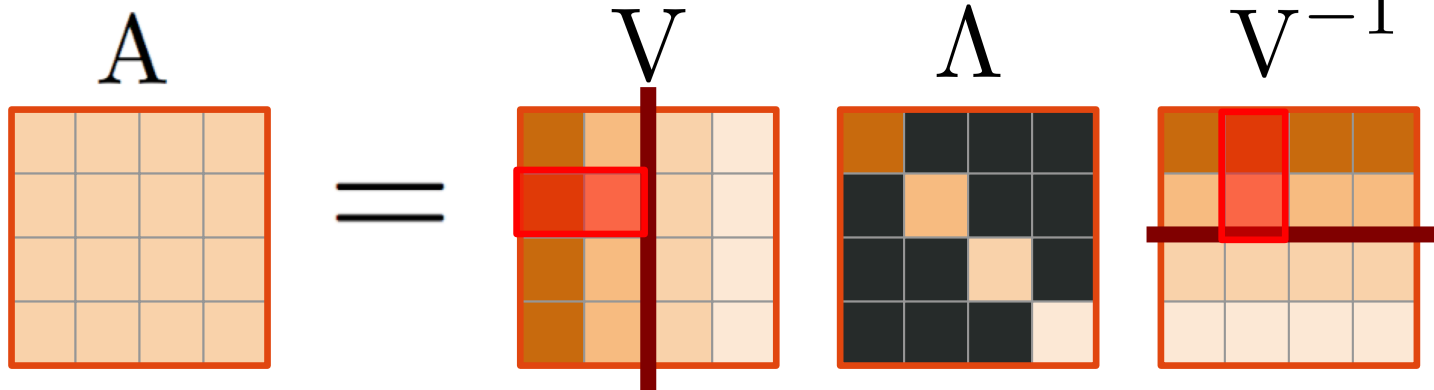
- Fundamental limits of sampling strategies
  - Minmax recovery error
  - Lower bound
  - Sampling algorithm
  - Upper bound



Optimal sampling distribution depends on properties of graph Fourier

$$\pi_i \propto \sqrt{\sum_{k=1}^{\kappa} \left(V_{k,i}^{-1}\right)^2 \sum_{k=1}^{\kappa} (V_{i,k})^2}$$

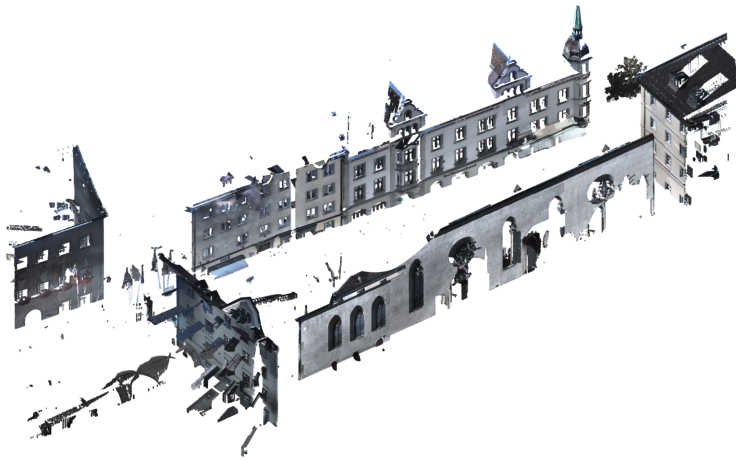
$\Lambda$                        $V^{-1}$



# GSP: Sampling & recovery

## Applications

- Resampling of 3D point clouds

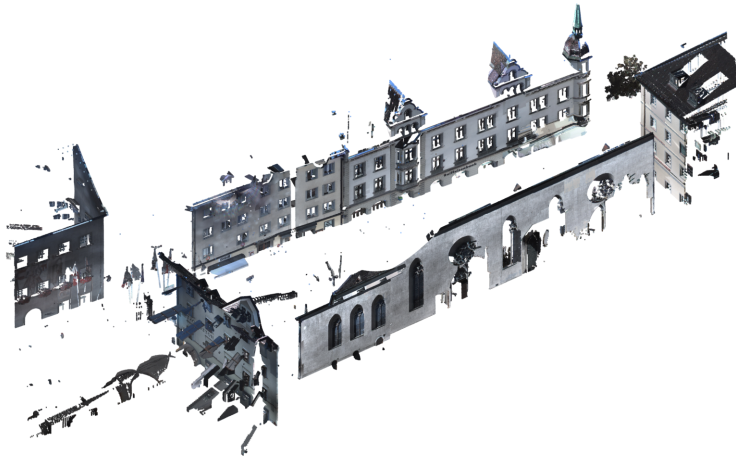


Over 30 million 3D points

# GSP: Sampling & recovery

## Applications

- Resampling of 3D point clouds



Over 30 million 3D points

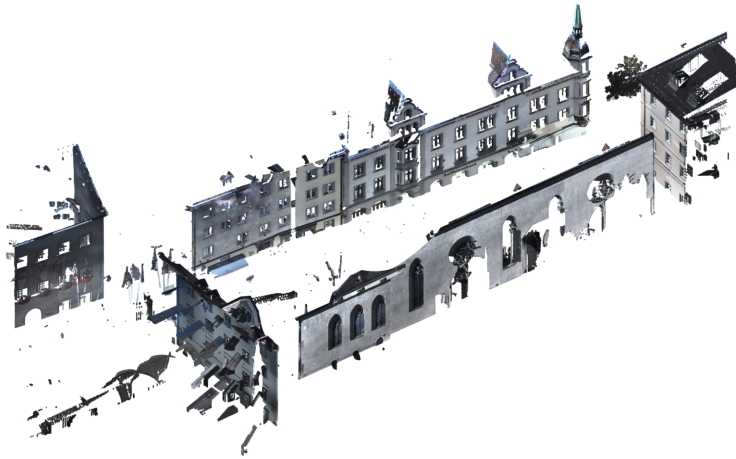


uniform sampling (1000)

# GSP: Sampling & recovery

## Applications

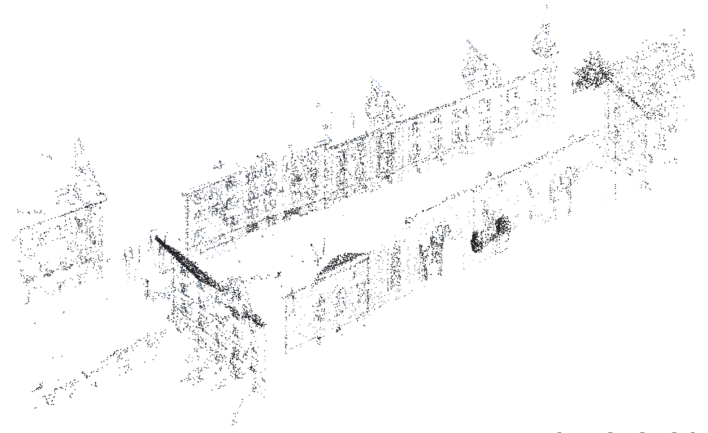
- Resampling of 3D point clouds



Over 30 million 3D points



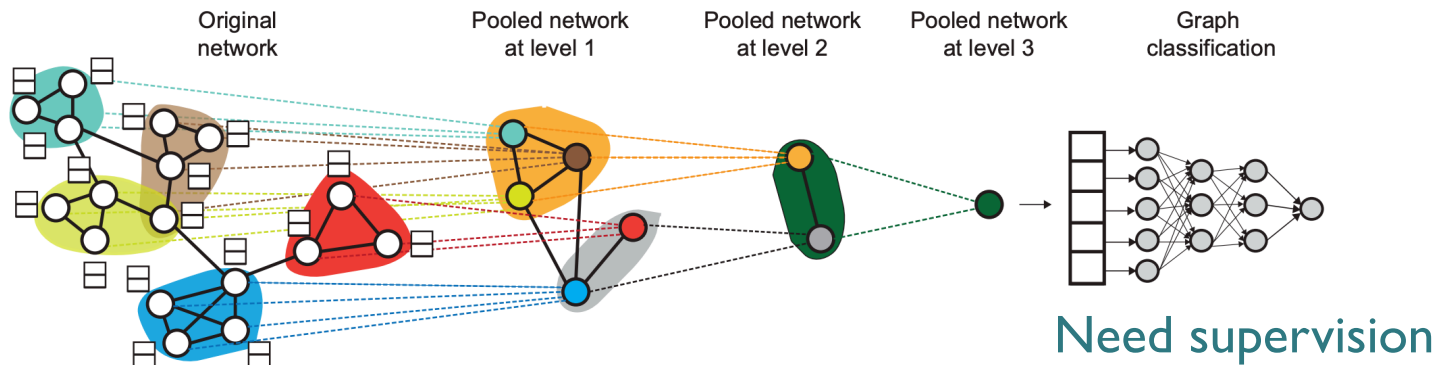
uniform sampling (1000)



designed sampling (1000)

# GNN: Sampling & recovery

## Diffpool: Graph pooling in multiscale graph neural network



*Trainable* sampling operator

$$\Psi = \text{softmax}(\text{GNN}(A, \mathbf{x}))$$

Data pooling

$$\mathbf{x}' = \Psi \mathbf{x}$$

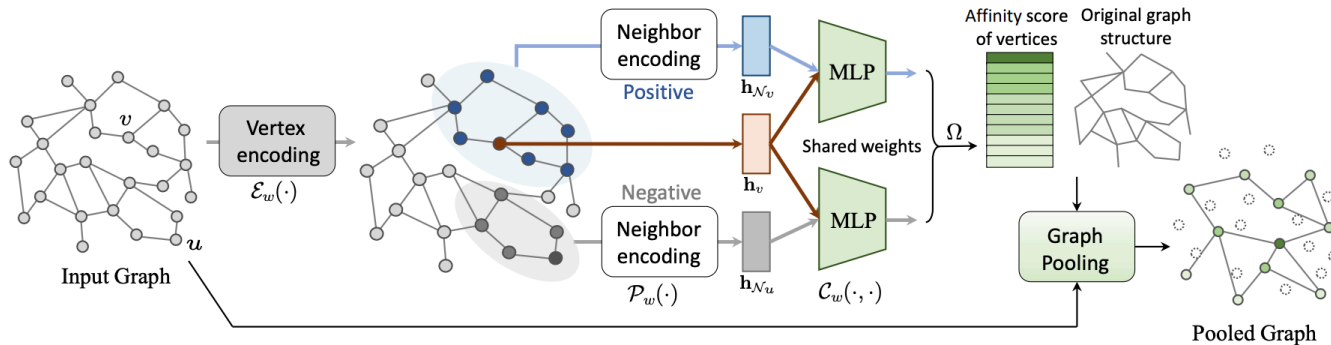
Structure pooling

$$A' = \Psi A \Psi^T$$



# GNN: Sampling & recovery

## Proposed graph pooling in multiscale graph neural network



Self-supervision / supervision

$$\max_{\mathcal{M} \subset \mathcal{V}} C(\mathcal{M}), \quad \text{subject to} \quad |\mathcal{M}| = M.$$

### Vertex-selection criterion


$$\begin{aligned} C(\mathcal{M}) &= I^{(\mathcal{M})}(\mathbf{v}, \mathbf{n}) = D_{\text{KL}}(P_{\mathbf{v}, \mathbf{n}} \| P_{\mathbf{v}} \otimes P_{\mathbf{n}}) \\ &\geq \sup_{T \in \mathcal{T}} \left\{ \mathbb{E}_{\mathbf{s}_v, \mathbf{q}_{N_v} \sim P_{\mathbf{v}, \mathbf{n}}} [T(\mathbf{s}_v, \mathbf{q}_{N_v})] - \mathbb{E}_{\mathbf{s}_v \sim P_{\mathbf{v}}, \mathbf{q}_{N_u} \sim P_{\mathbf{n}}} [e^{T(\mathbf{s}_v, \mathbf{q}_{N_u}) - 1}] \right\} \end{aligned}$$

GNN
node feature
neighborhood feature

# GNN: Sampling & recovery

## Experimental results


- Graph classification

Dataset	IMDB-B	IMDB-M	COLLAB	D&D	PROTEINS	ENZYMES
# Graphs (Classes)	1000 (2)	1500 (3)	5000 (3)	1178 (2)	1113 (2)	600 (6)
Avg. # Vertices	19.77	13.00	74.49	284.32	39.06	32.63
PatchySAN [34]	$76.27 \pm 2.6$	$69.70 \pm 2.2$	$43.33 \pm 2.8$	$72.60 \pm 2.2$	$75.00 \pm 2.8$	-
ECC [40]	-	-	67.79	72.54	72.65	53.50
Set2Set [20]	-	-	71.75	78.12	74.29	60.15
DGCNN [49]	$70.00 \pm 0.9$	$47.83 \pm 0.9$	$73.76 \pm 0.5$	$79.37 \pm 0.9$	$73.68 \pm 0.9$	-
DiffPool [46]	70.40	47.83	75.84	80.64	76.25	62.53
Graph U-Net [19]	72.10	48.33	77.56	82.43	77.68	58.57
SAGPool [28]	72.80	49.43	78.52	82.84	78.28	60.23
AttPool [24]	73.60	50.67	77.04	79.20	76.50	59.76
StructPool [47]	74.70	52.47	74.22	84.19	80.36	<b>63.83</b>
 GXN	<b><math>77.30 \pm 0.8</math></b>	<b><math>54.57 \pm 0.9</math></b>	<b><math>80.62 \pm 0.8</math></b>	<b><math>84.26 \pm 1.3</math></b>	<b><math>80.38 \pm 1.2</math></b>	$60.43 \pm 1.0$

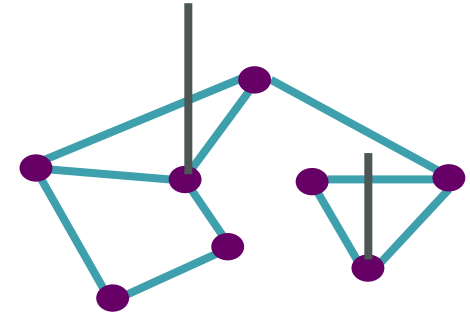
# GNN: Sampling & recovery

## Experimental results

- Node classification

Dataset # Vertices (Classes) Supervision	Cora 2708 (7)		Citeseer 3327 (6)		Pubmed 19717 (3)	
	full-sup.	semi-sup.	full-sup.	semi-sup.	full-sup.	semi-sup.
DeepWalk [36]	$78.4 \pm 1.7$	$67.2 \pm 2.0$	$68.5 \pm 1.8$	$43.2 \pm 1.6$	$79.8 \pm 1.1$	$65.3 \pm 1.1$
ChebNet [10]	$86.4 \pm 0.5$	$81.2 \pm 0.5$	$78.9 \pm 0.4$	$69.8 \pm 0.5$	$88.7 \pm 0.3$	$74.4 \pm 0.4$
GCN [27]	$86.6 \pm 0.4$	$81.5 \pm 0.5$	$79.3 \pm 0.5$	$70.3 \pm 0.5$	$90.2 \pm 0.3$	$79.0 \pm 0.3$
GAT [43]	$87.8 \pm 0.7$	$83.0 \pm 0.7$	$80.2 \pm 0.6$	$73.5 \pm 0.7$	$90.6 \pm 0.4$	$79.0 \pm 0.3$
FastGCN [7]	$85.0 \pm 0.8$	$80.8 \pm 1.0$	$77.6 \pm 0.8$	$69.4 \pm 0.8$	$88.0 \pm 0.6$	$78.5 \pm 0.7$
ASGCN [25]	$87.4 \pm 0.3$	-	$79.6 \pm 0.2$	-	$90.6 \pm 0.3$	-
Graph U-Net [19]	-	84.4	-	73.2	-	79.6
 GXN	<b><math>88.9 \pm 0.4</math></b>	<b><math>85.1 \pm 0.6</math></b>	<b><math>80.9 \pm 0.4</math></b>	<b><math>74.8 \pm 0.4</math></b>	<b><math>91.8 \pm 0.3</math></b>	<b><math>80.2 \pm 0.3</math></b>

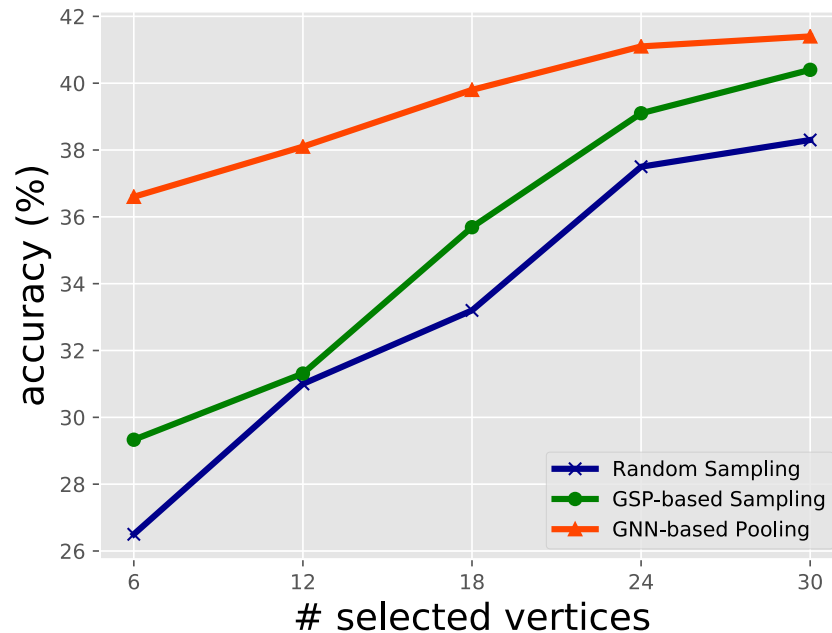
# GNN: Sampling & recovery



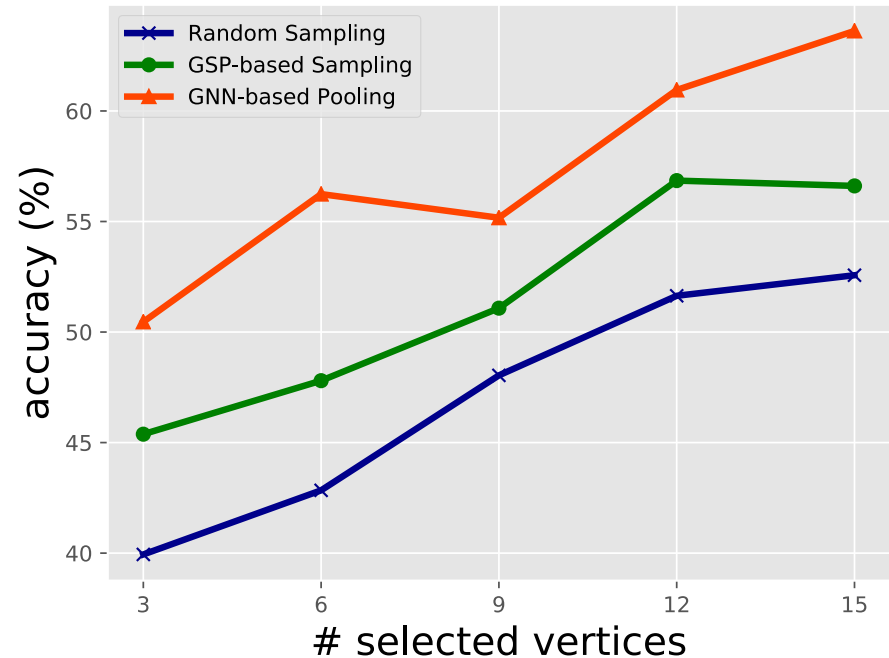
## Experimental results

- Active-sampling-based semi-supervised learning

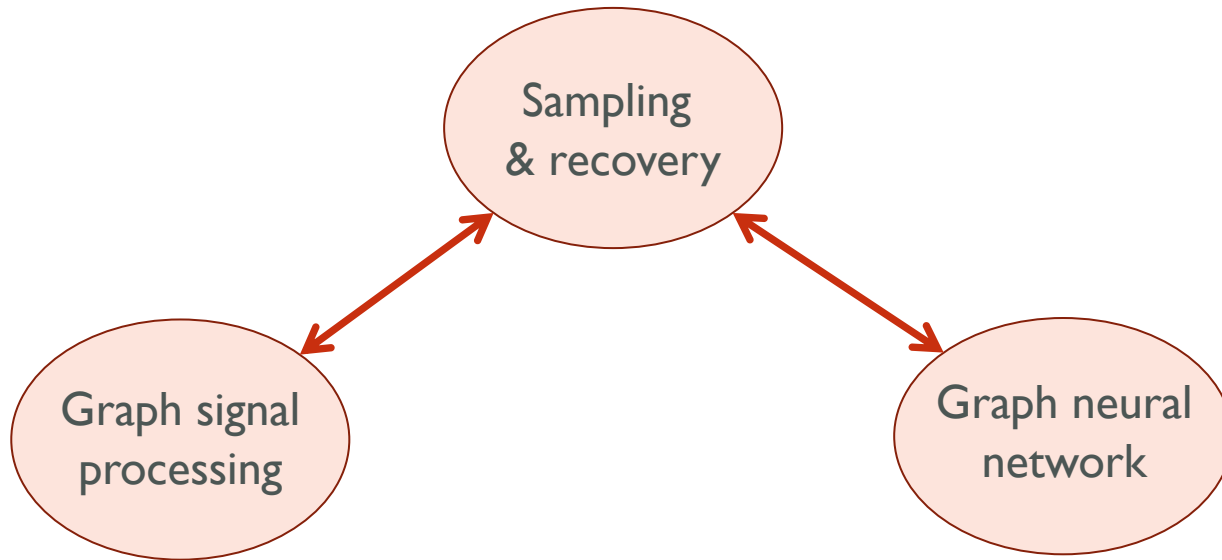
## Citeseer: 3327 nodes



## Pubmed: 19717 nodes



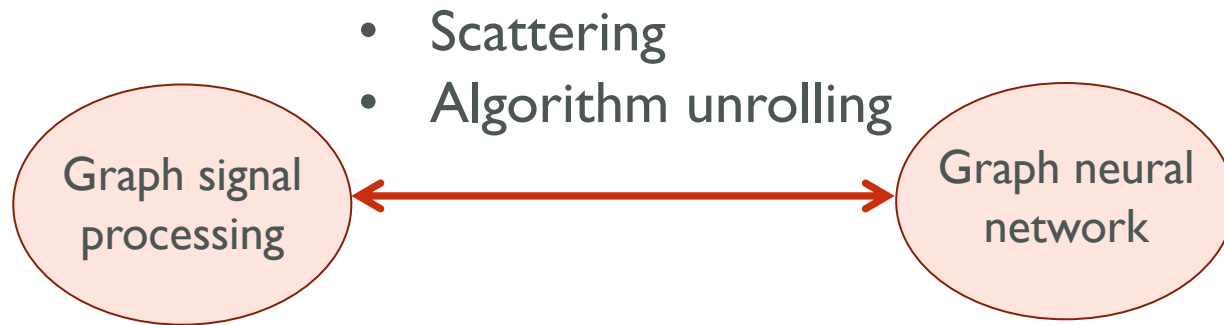
# Bridging GSP and GNN



# Bridging GSP and GNN



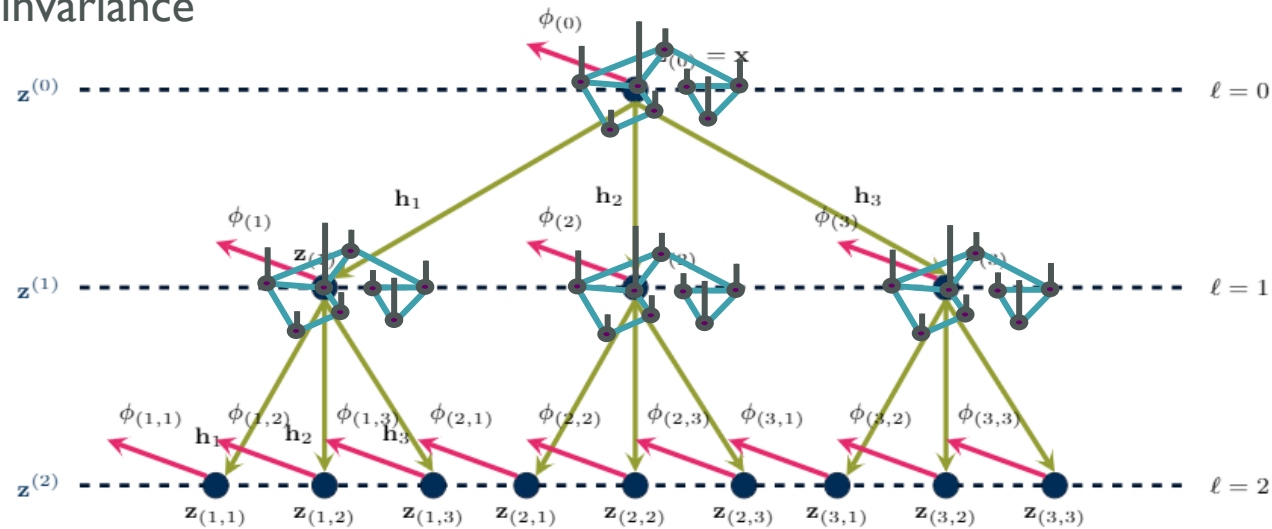
# Bridging GSP and GNN



# Graph scattering transforms

Graph scattering transforms are **nontrainable** GCNs

- Parameters of the graph convolutions are mathematically designed
- Theoretical property
  - Energy preservation
  - Permutation invariance
  - Stability



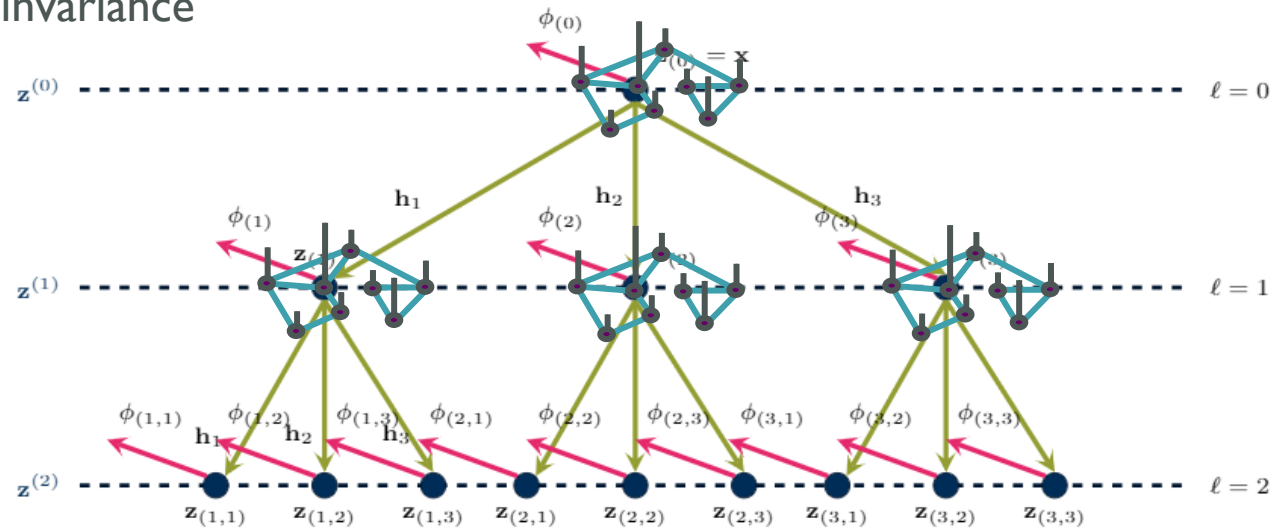
- Dongmian Zou, Gilad Lerman, "Graph Convolutional Neural Networks via Scattering", Applied and Computational Harmonic Analysis, 2019
- Fernando Gama, Alejandro Ribeiro, Joan Bruna, "Diffusion Scattering Transforms on Graphs" ICLR, 2019



# Graph scattering transforms

Graph scattering transforms are **nontrainable** GCNs

- Parameters of the graph convolutions are mathematically designed
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  - Energy preservation
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**Scattering => exponential growth!**

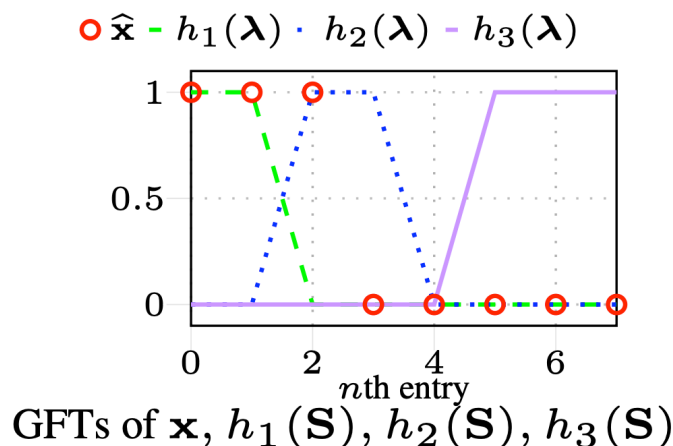
- Dongmian Zou, Gilad Lerman, "Graph Convolutional Neural Networks via Scattering", Applied and Computational Harmonic Analysis, 2019
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# Graph scattering transforms

Main idea: a **pruning** framework to select informative features of the graph scattering transforms

- Optimal pruning

$$\begin{aligned} \max_{\{f_{(p,j)}\}_{j=1}^J} \quad & \sum_{j=1}^J \left( \sum_{n=1}^N \left( \hat{h}_j(\lambda_n)^2 - \tau \right) [\hat{\mathbf{z}}_{(p)}]_n^2 \right) f_{(p,j)} \\ \text{s. t.} \quad & f_{(p,j)} \in \{0, 1\}, \quad j = 1, \dots, J \end{aligned}$$

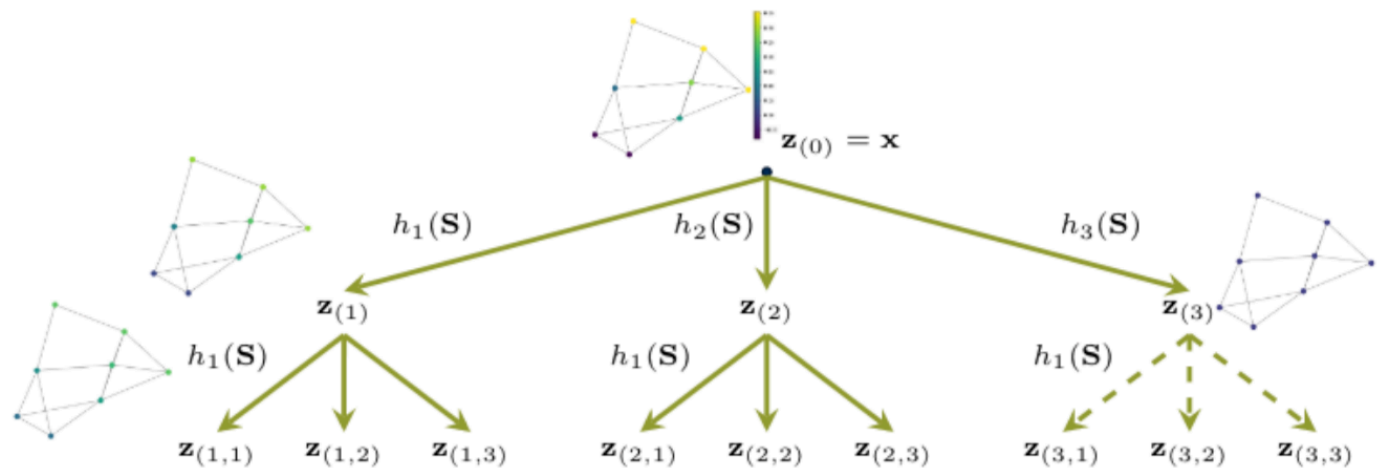


# Graph scattering transforms

Main idea: a **pruning** framework to select informative features of the graph scattering transforms

- Optimal pruning

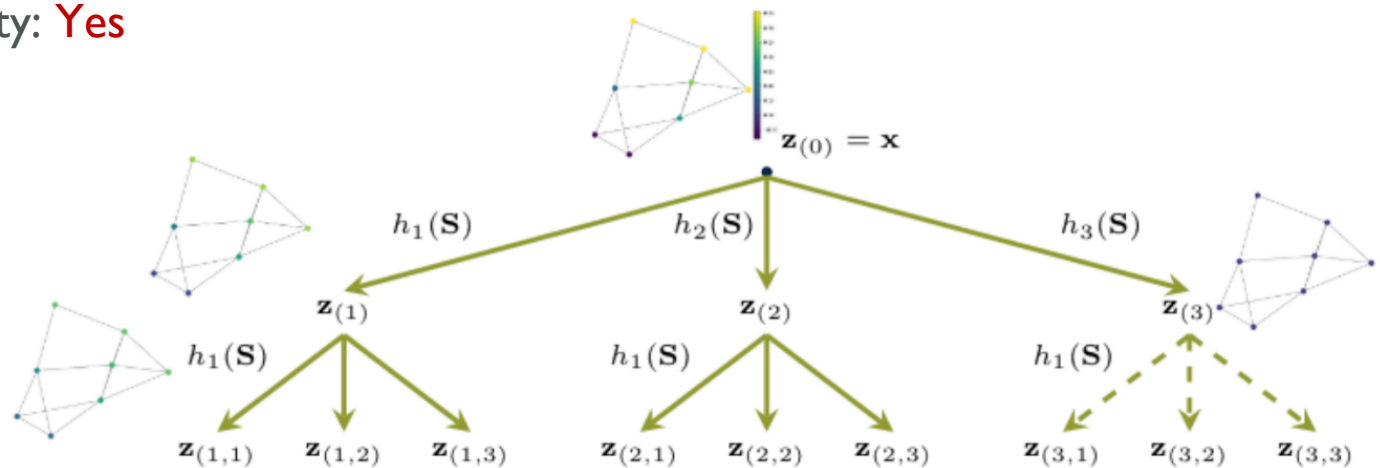
$$f_{(p,j)}^* = \begin{cases} 1 & \text{if } \frac{\|\mathbf{z}_{(p,j)}\|^2}{\|\mathbf{z}_{(p)}\|^2} > \tau, \\ 0 & \text{if } \frac{\|\mathbf{z}_{(p,j)}\|^2}{\|\mathbf{z}_{(p)}\|^2} < \tau. \end{cases}, j = 1, \dots, J$$



# Graph scattering transforms

Main idea: a **pruning** framework to select informative features of the graph scattering transforms

- Optimal pruning
- Theoretical property
  - Energy preservation: **No**
  - Permutation invariance: **?**
  - Stability: **Yes**



# Graph scattering transforms

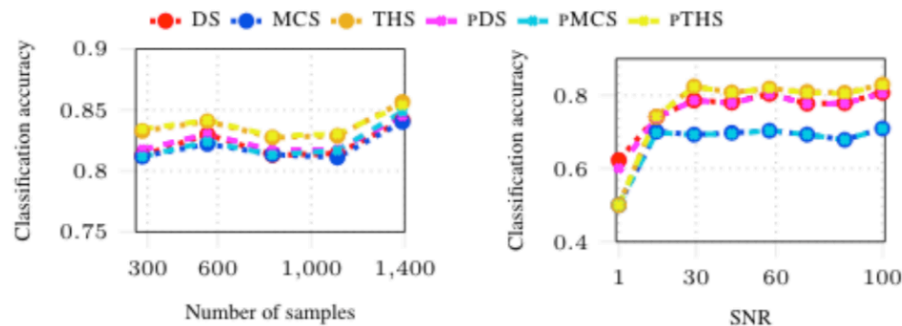
Main idea: a **pruning** framework to select informative features of the graph scattering transforms

	Method	Data Set			
		ENZYMES	D&D	COLLAB	PROTEINS
Kernel	SHORTEST-PATH	42.32	78.86	59.10	76.43
	WL-OA	60.13	79.04	80.74	75.26
GNNs	PATCHYSAN	–	76.27	72.60	75.00
	GRAPHSAGE	54.25	75.42	68.25	70.48
	ECC	53.50	74.10	67.79	72.65
	SET2SET	60.15	78.12	71.75	74.29
	SORTPOOL	57.12	79.37	73.76	75.54
	DIFFPOOL-DET	58.33	75.47	<b>82.13</b>	75.62
	DIFFPOOL-NO LP	62.67	79.98	75.63	77.42
	DIFFPOOL	<b>64.23</b>	81.15	75.50	78.10
Scattering	GSC	53.88	76.57	76.88	74.03
	GST	59.84	79.28	77.32	76.23
	PGST (Ours)	60.25	<b>81.27</b>	78.40	<b>78.57</b>

Mathematically designed framework is comparable with trained framework

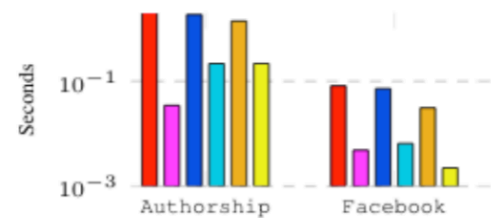
# Graph scattering transforms

Main idea: a **pruning** framework to select informative features of the graph scattering transforms



(a) Authorship

(b) Facebook

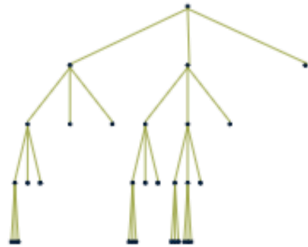


(c) Runtime

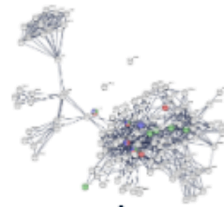
Similar performance, but 10 times faster!

# Graph scattering transforms

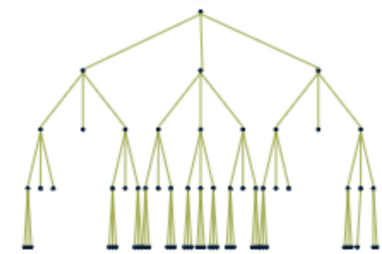
Main idea: a **pruning** framework to select informative features of the graph scattering transforms



(a) Academic collaboration



(b) Protein-protein network

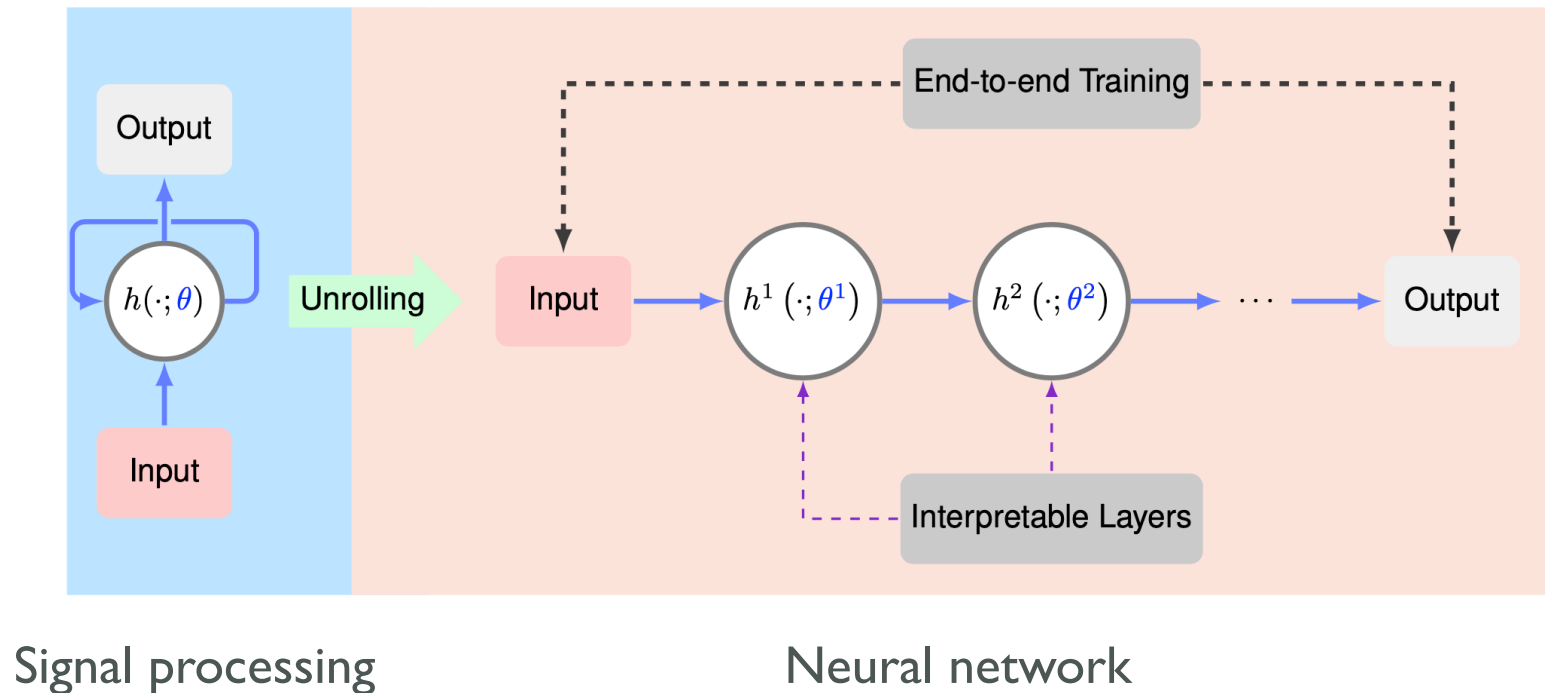


(c) 3D point cloud

**Pruning pattern reflects the complexity of dataset**

# Graph unrolling networks

Algorithm unrolling framework: Transform an iterative algorithm to a multilayer neural network

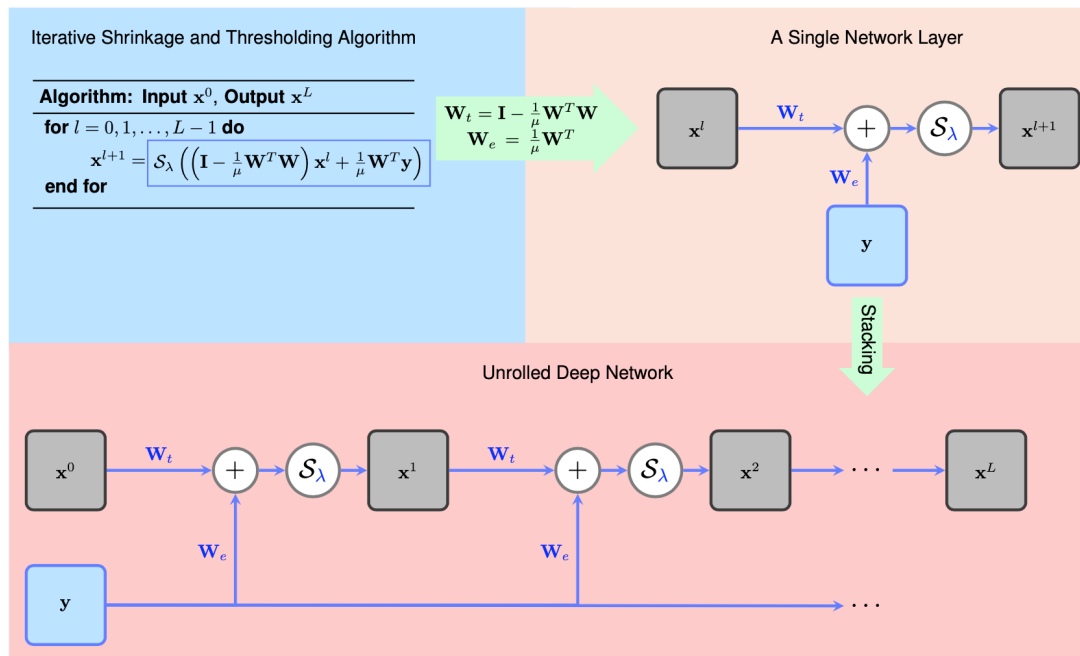




# Graph unrolling networks

Algorithm unrolling framework: Transform an iterative algorithm to a multilayer neural network

**Sparse coding**  $\min_{\mathbf{x}} \frac{1}{2} \|\mathbf{y} - \mathbf{W} \mathbf{x}\|_2^2 + \lambda \|\mathbf{x}\|_1$



# Graph unrolling networks

Algorithm unrolling framework: Transform an iterative algorithm to a multilayer neural network

$$\min_{\mathbf{s} \in \mathbb{R}^N} \frac{1}{2} \|\mathbf{t} - \mathbf{x}\|_2^2 + u(\mathbf{y}) + r(\mathbf{z}),$$

subject to  $\mathbf{x} = \mathbf{h} *_{\mathbf{v}} \mathbf{s}, \quad \mathbf{y} = \mathbf{P} \mathbf{x}, \quad \mathbf{z} = \mathbf{Q} \mathbf{s}$

Analytical iterative solution

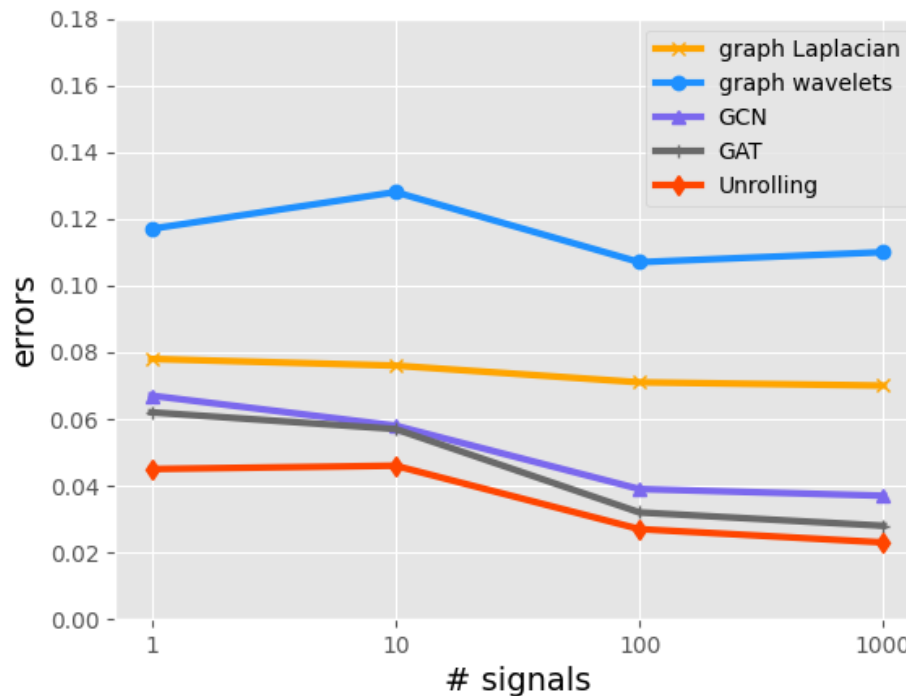
One network layer

$\mathbf{x} \leftarrow \tilde{\mathbf{P}} \left( \mu_1 \mathbf{h} *_{\mathbf{v}} \mathbf{s} + \mathbf{t} + \mu_2 \mathbf{P}^T \mathbf{y} \right),$	$\longleftrightarrow$	$\mathbf{x} \leftarrow \mathbb{A} *_{\mathbf{a}} \mathbf{s} + \mathbb{B} *_{\mathbf{a}} \mathbf{t} + \mathbb{C} *_{\mathbf{a}} (\mathbf{P}^T \mathbf{y})$
$\mathbf{s} \leftarrow \tilde{\mathbf{Q}} \left( \mu_1 \mathbf{h} *_{\mathbf{v}}^T \mathbf{x} + \mu_3 \mathbf{Q}^T \mathbf{z} \right),$	$\longleftrightarrow$	$\mathbf{s} \leftarrow \mathbb{D} *_{\mathbf{a}} \mathbf{x} + \mathbb{E} *_{\mathbf{a}} (\mathbf{Q}^T \mathbf{z})$
$\mathbf{y} \leftarrow \arg \min_{\mathbf{y}} \frac{\mu_2}{2} \ \mathbf{y} - \mathbf{P} \mathbf{x}\ _2^2 + u(\mathbf{y}),$	$\longleftrightarrow$	$\mathbf{y} \leftarrow \text{NN}_u (\mathbf{P} \mathbf{x})$
$\mathbf{z} \leftarrow \arg \min_{\mathbf{z}} \frac{\mu_3}{2} \ \mathbf{z} - \mathbf{Q} \mathbf{s}\ _2^2 + r(\mathbf{z}),$	$\longleftrightarrow$	$\mathbf{z} \leftarrow \text{NN}_r (\mathbf{Q} \mathbf{s})$

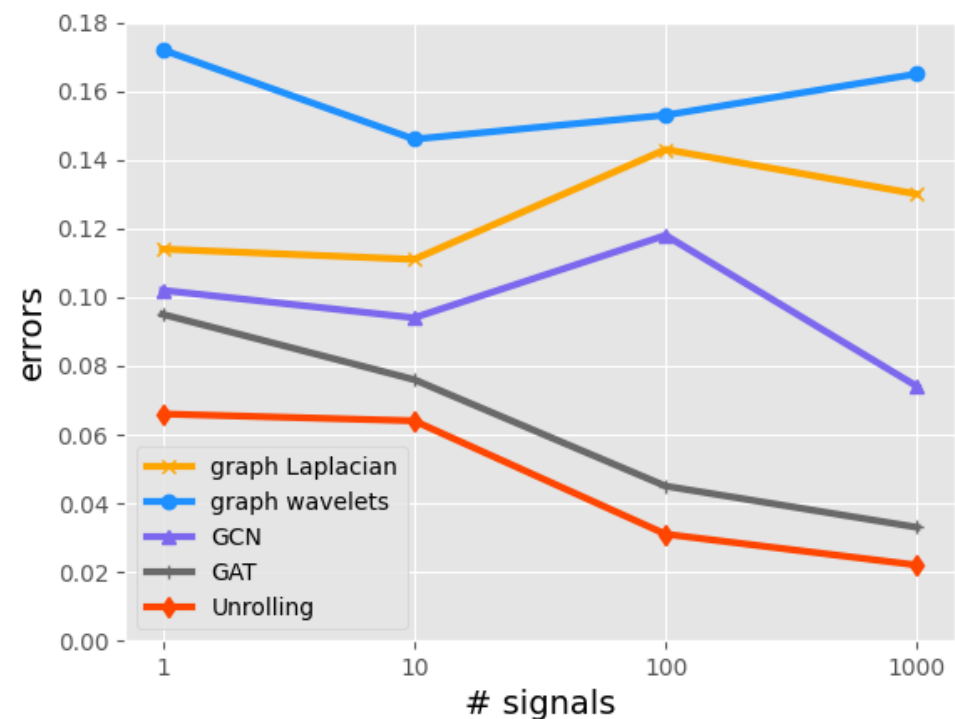
# Graph unrolling networks

## Denoising of graph-structured data

### Smooth graph signals



### Piecewise-smooth graph signals



# Conclusions

## Graph-structured data science

- Graph signal processing (GSP)
- Graph neural network (GNN)

## Sampling and recovery of graph-structured data

- GSP: Mathematically designed graph sampling operator
- GNN: Trainable graph pooling operator

## Bridging GSP and GNN

- Graph scattering transform
- Graph unrolling network

Thank you!