AdaGNN: Graph Neural Networks with Adaptive Frequency Response Filter

Yushun Dong[1], Kaize Ding[2], Brian Jalaian[3], Shuiwang Ji[4], Jundong Li[1]

[1]University of Virginia, [2]Arizona State University, [3]Army Research Laboratory, [4]Texas A&M University

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Overview

Background Introduction

Previous Works

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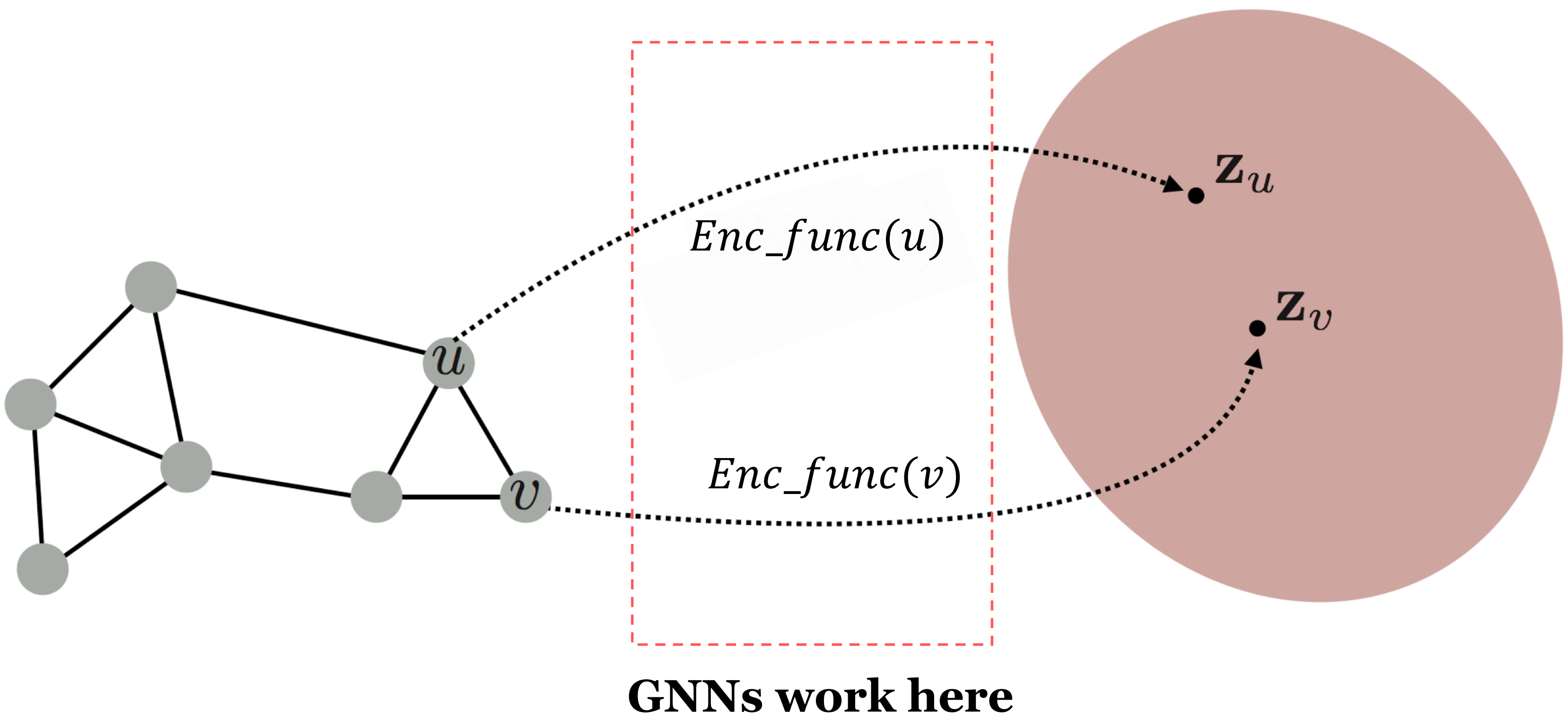
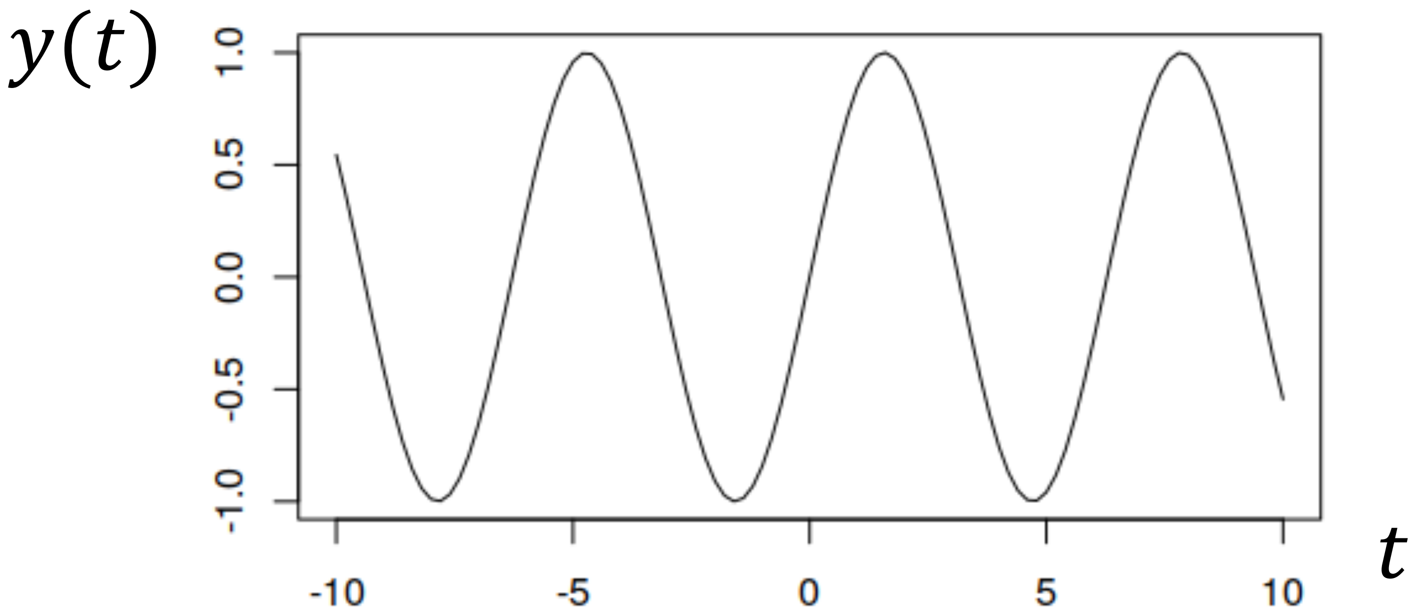
Future Works

Goal of Graph Neural Networks (GNNs): to encode nodes so that similarity in the embedding space (e.g., dot product) approximates similarity in the original network.



Background Introduction: Frequency in Graphs

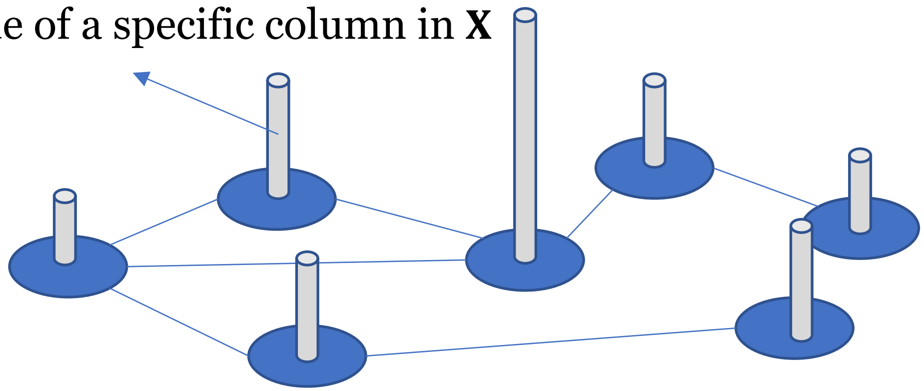
Traditionally, frequency is defined as the number of occurrences of a repeating event per unit of time*, and a basic unit of frequency is Hertz.



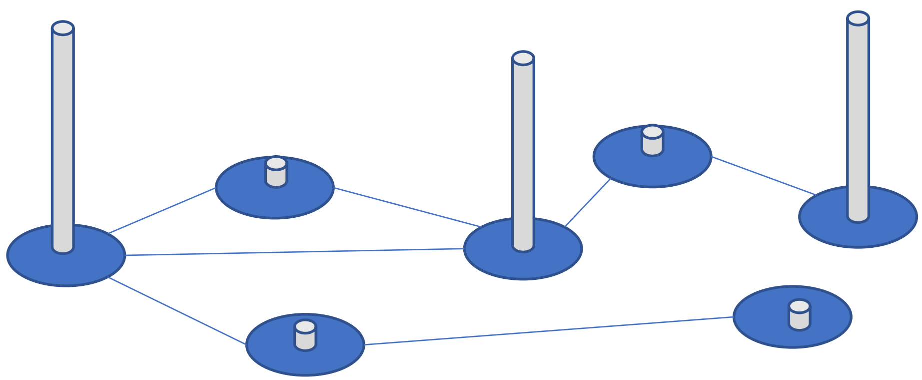
* https://en.wikipedia.org/wiki/Frequency

Background Introduction: Frequency in Graphs

In graphs, we generalize the notion of frequency in the spatial domain to measure how fast a signal changes w.r.t. its graph structure.

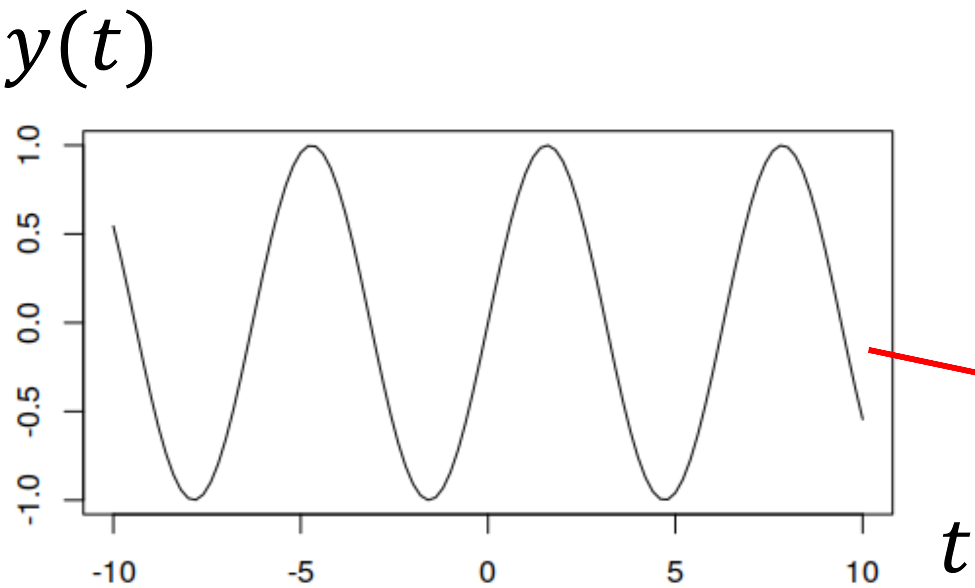


Low frequency: the signal changes slowly across edges.

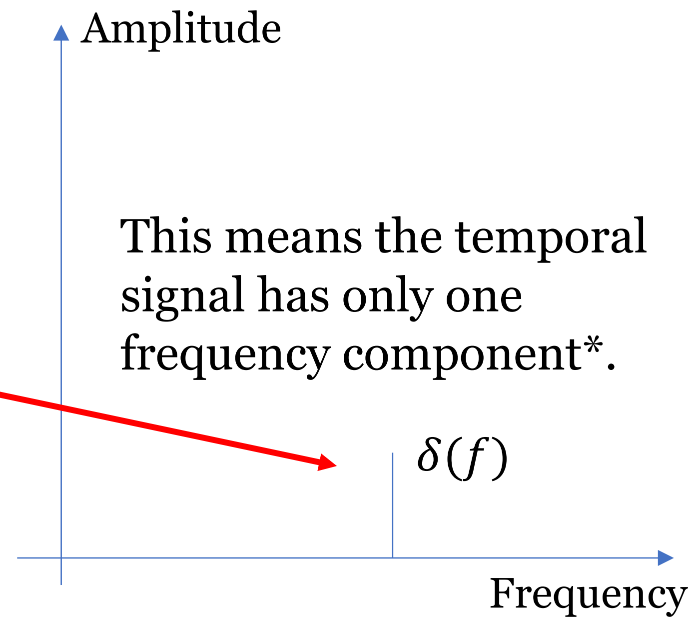


High frequency: the signal changes fast across edges.

For time series signals, we have frequency basis. Cosine function is a commonly utilized basis for time series signal. For example, it is utilized as one of the basis of Fourier Transform.



Time domain



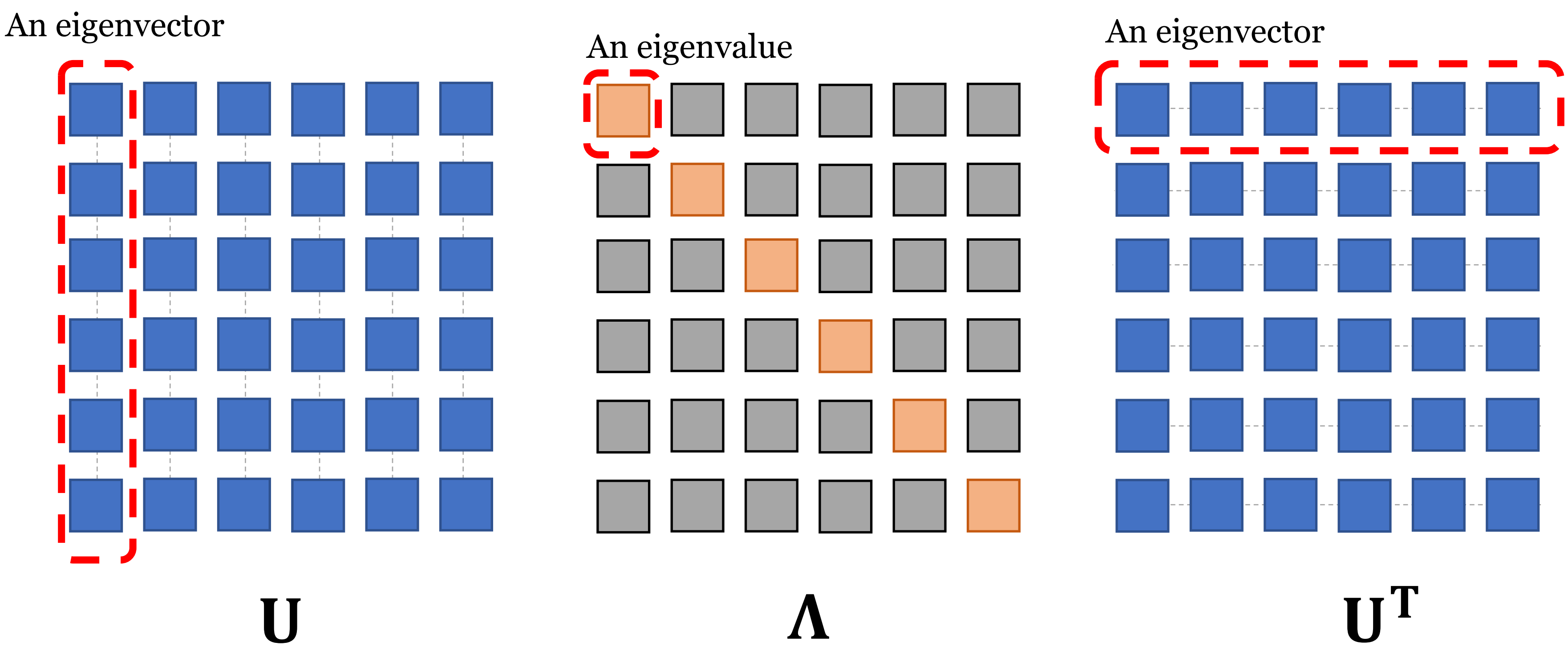
Frequency domain

*Here we only show the positive half axis in the frequency domain.

Background Introduction: Frequency in Graphs

In graphs, we utilize the eigenvectors of graph Laplacian as the basis of different frequencies*.

$$\mathbf{L} = \mathbf{D} - \mathbf{A} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^{\mathbf{T}}$$



*Here the frequency notion is defined based on graph Laplacian. Similar notion can also be defined based on adjacency matrix, but larger eigenvalues corresponds to lower frequencies.

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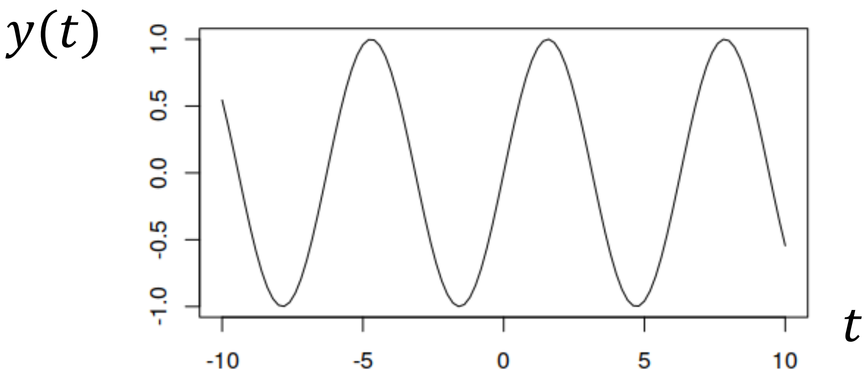
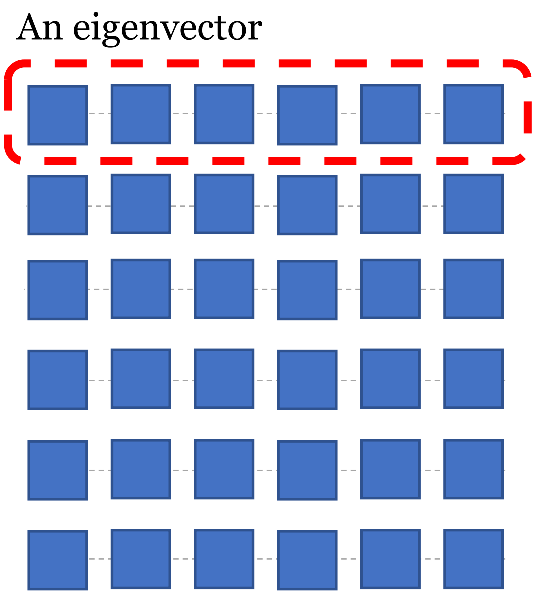
We can intuitively understand the functionality of the graph Laplacian eigenvectors as cosine functions.

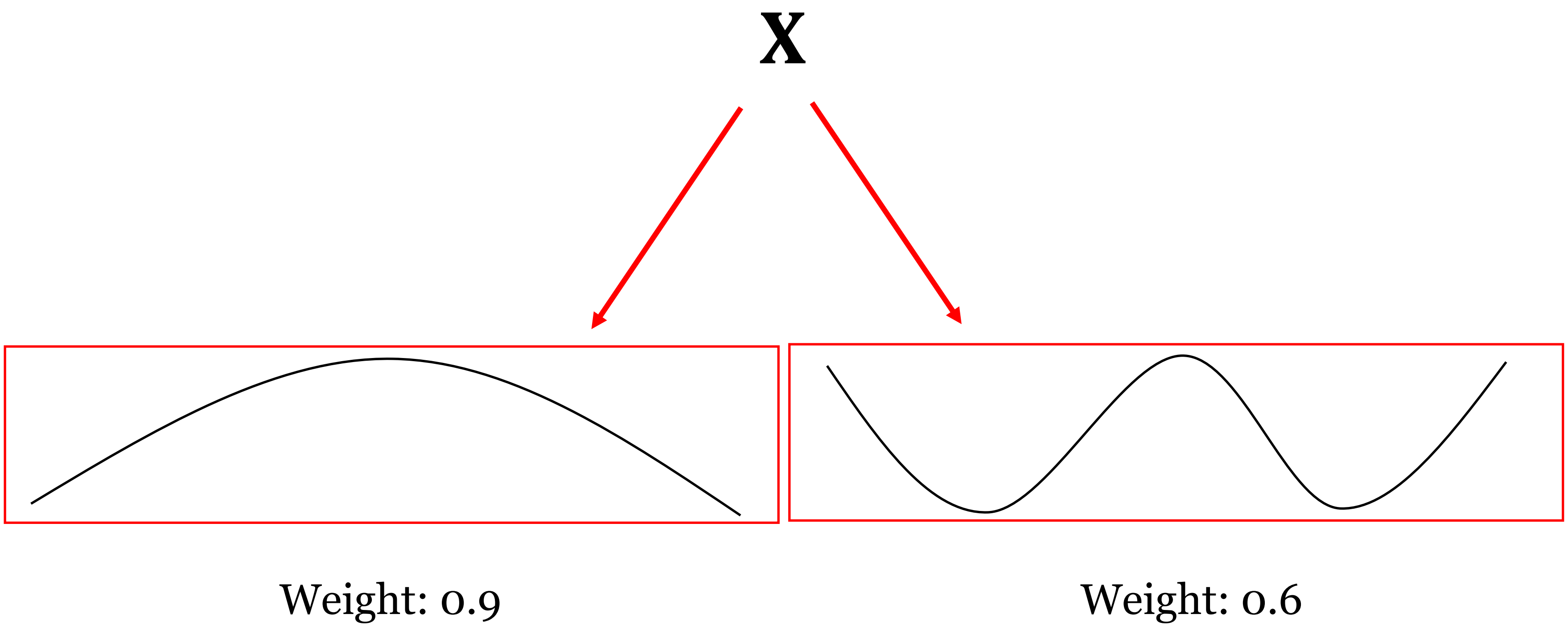




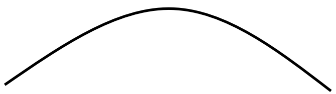
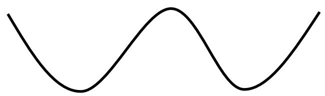
The corresponding eigenvalue is the frequency.

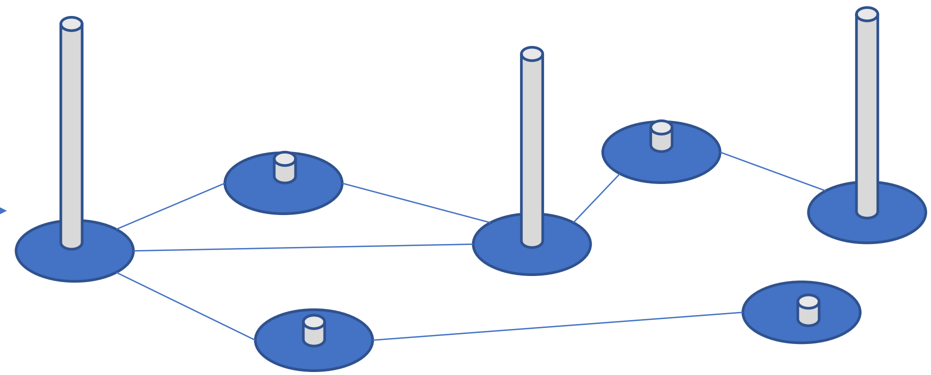
Background Introduction: Graph (low-pass) Filtering

By projecting **X** on different eigenvectors:



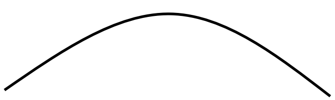
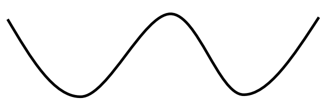
Background Introduction: Graph (low-pass) Filtering

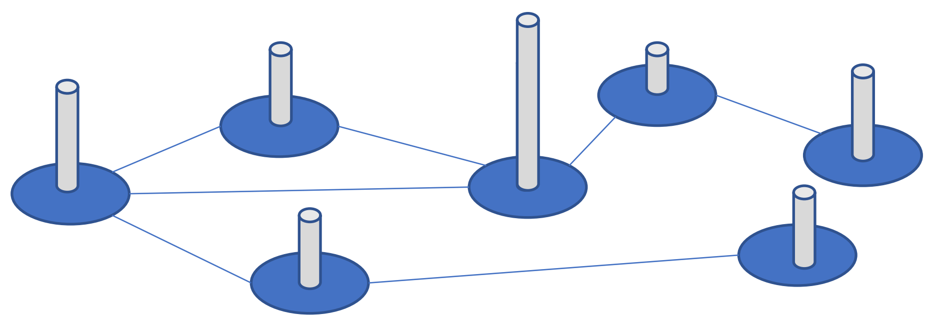
0.9	0.6
	



Eigenvectors (of graph Laplacian) are regarded as signal basis.

Graph Filter

0.9	0.2
	



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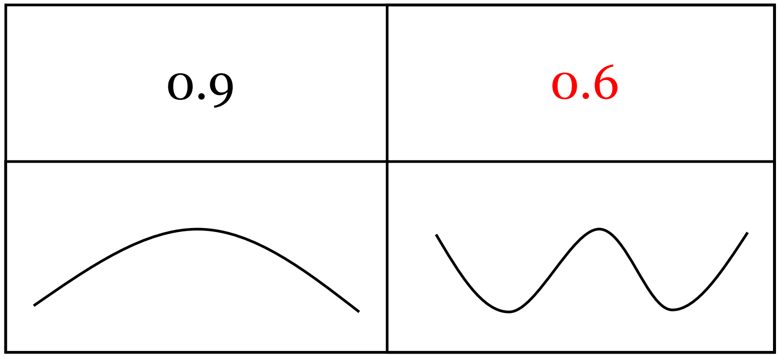
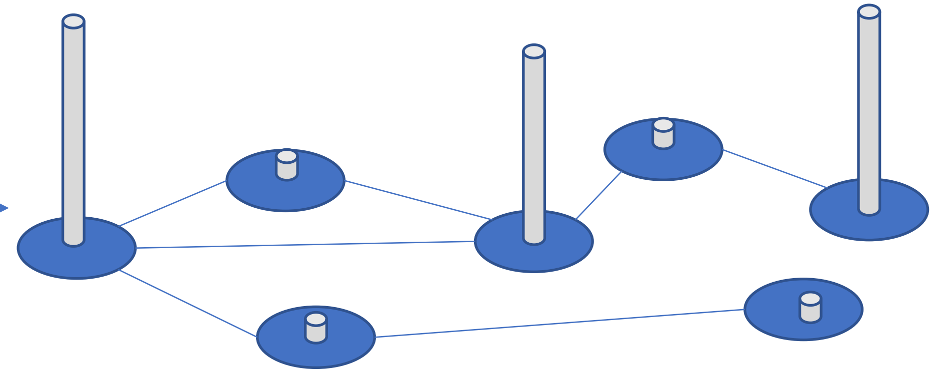
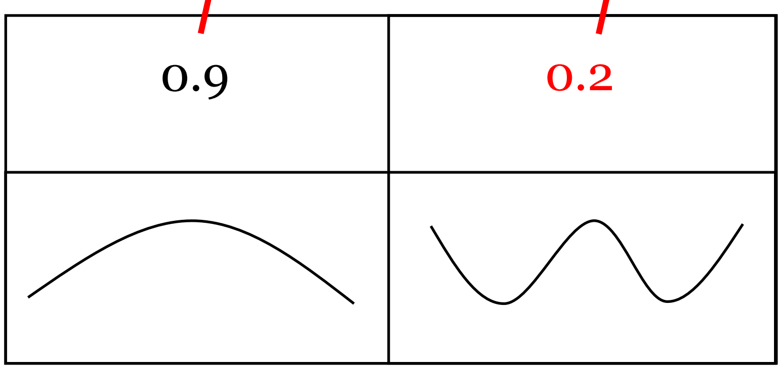
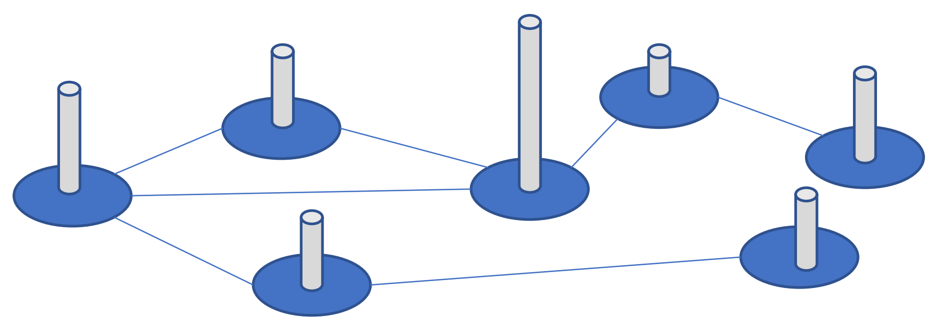




Graph Filter

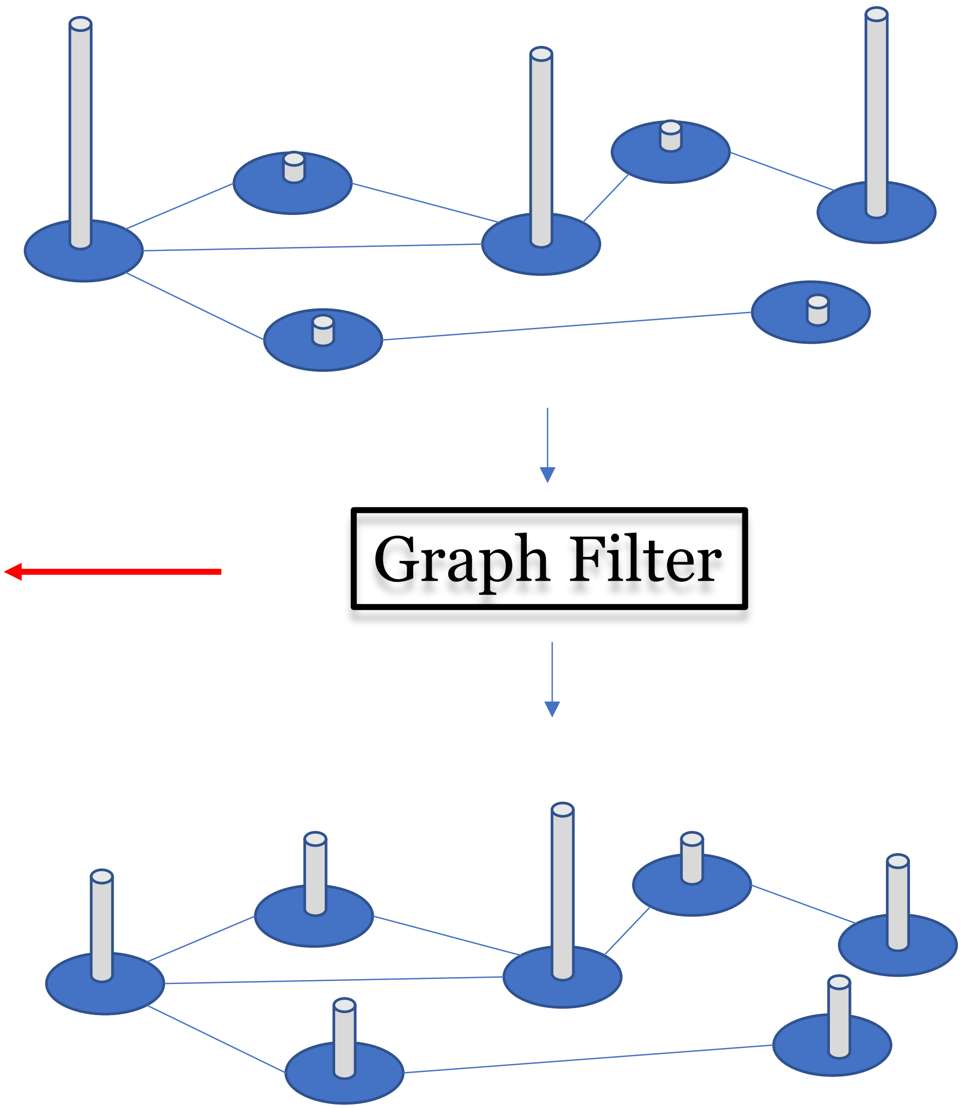
Re-weighted components **X** projected on each basis.





Background Introduction: Graph (low-pass) Filtering

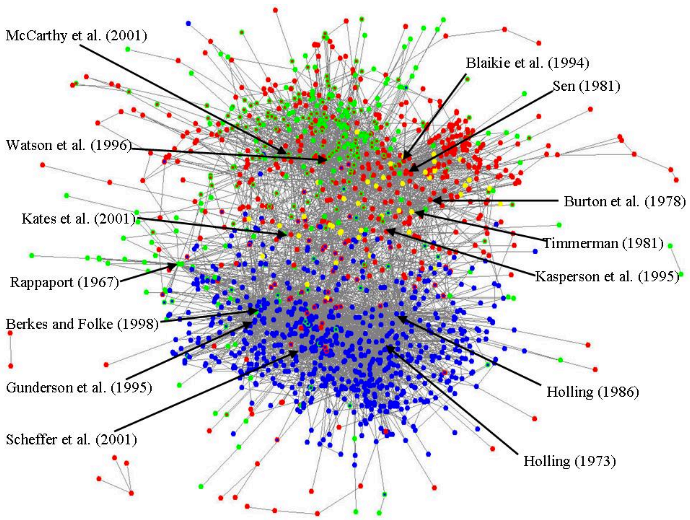
Graph (low-pass) filtering is a process of reducing the weight on eigenvector basis corresponding to large eigenvalues (of the graph Laplacian matrix) in the graph signal (i.e., **X** given **A**).



Background Introduction: Graph (low-pass) Filtering

Why we need to do this?

By filtering out "high-frequency" information (i.e., signals with high variances across the graph), the neighbor nodes are made to be similar. This helps us capture the dependencies between linked nodes.



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Nevertheless, is low frequency all what we need?

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In assortative networks, similar nodes tend to link together; however, in disassortative networks, different nodes tend to link together.

This indicates that **only preserving low-frequency components cannot fully capture all useful information** [Bo et al. 2021].

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- Experiments & Conclusion
- Future Works

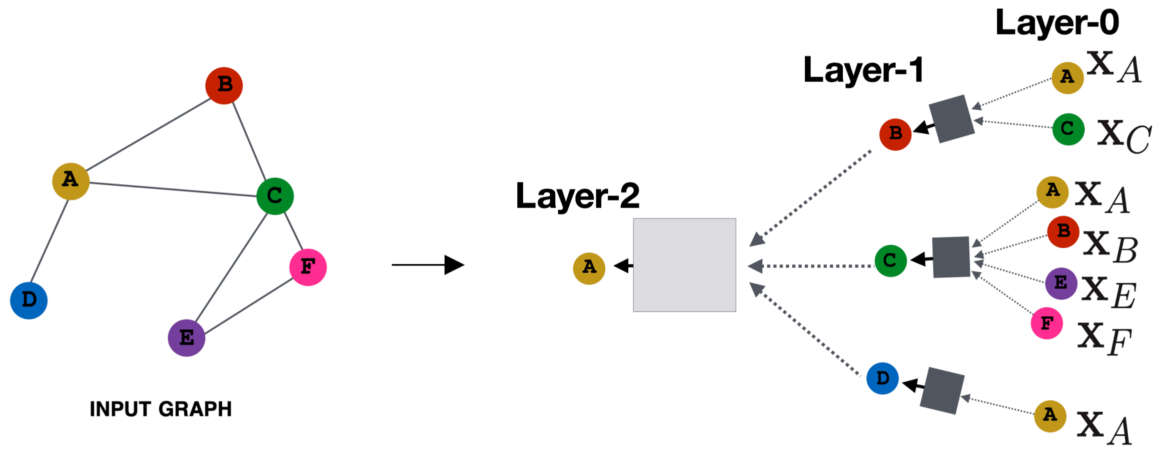
Previous Works: Spatial GNNs

Spatial GNNs: focus on information aggregation between nodes in the spatial domain;

Advantages: explainable and flexible;

Disadvantages: limited supporting theoretical basis; more of an empirical method;

Representative works: Graph Attention Network [Petar et al. 2017], GraphSAGE [Hamilton et al. 2017], etc.



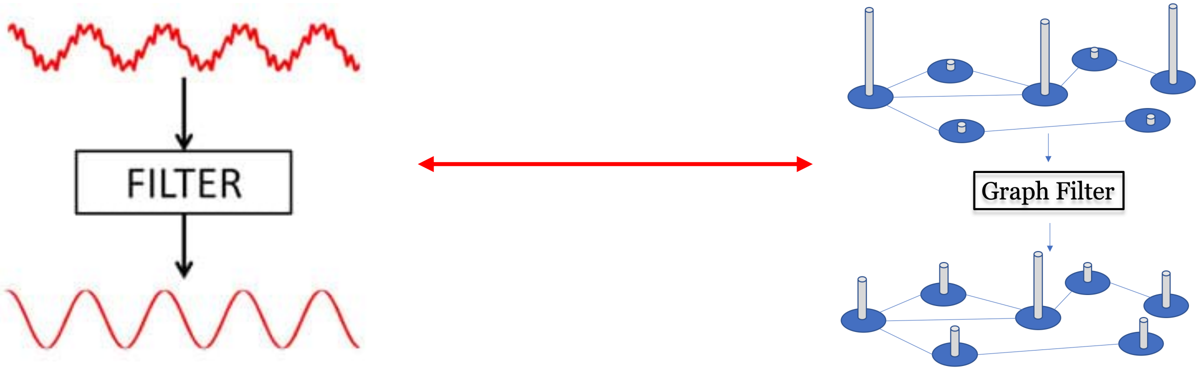
Previous Works: Spectral GNNs

Spectral GNNs: treat graph data as a whole and do signal filtering in the spectral domain;

Advantages: solid theoretical basis; easy to foresee the performance corresponding to certain type of graphs;

Disadvantages: hard to do inductive learning (not impossible though); low localized explainability;

Representative works: Fast Localized Graph Spectral Filtering [Defferrard et al. 2016], Graph Convolutional Network [Kipf et al. 2016], etc.



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Existing Problems: Non-learnable Graph Filter

We focus on the problems of spectral methods: existing models such as GCN can only achieve non-learnable graph filter, which means that it cannot adaptively capture useful information that is not contained in the low-frequency component;

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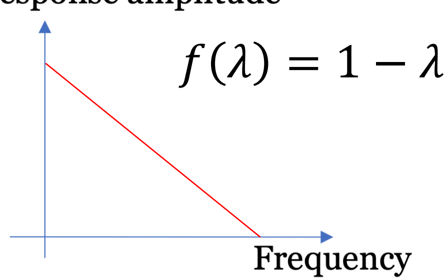
Layer expression of GCN:

$$\begin{aligned}\mathbf{Z} &= \sigma(\widetilde{\mathbf{D}}^{-\frac{1}{2}}\widetilde{\mathbf{A}}\widetilde{\mathbf{D}}^{-\frac{1}{2}}\mathbf{X}\mathbf{\Theta}) \\ &= \sigma[(\mathbf{I}-\tilde{\mathbf{L}})\mathbf{X}\mathbf{\Theta}] \\ &= \sigma[\mathbf{U}(\mathbf{I}-\mathbf{\Lambda})\mathbf{U}^{\mathrm{T}}\mathbf{X}\mathbf{\Theta}]\end{aligned}$$

Response amplitude



Frequency-response function

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\end{aligned}
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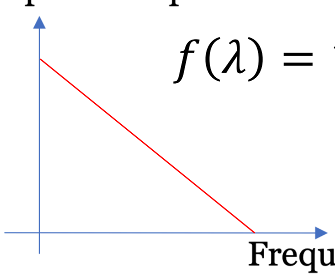
Response amplitude

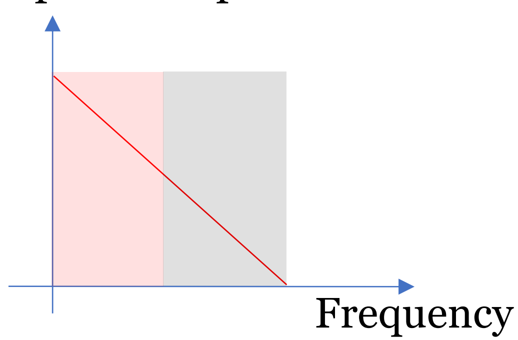
$$f(\lambda) = 1 - \lambda$$



Frequency-response function

Red component can be well-captured:

Response amplitude



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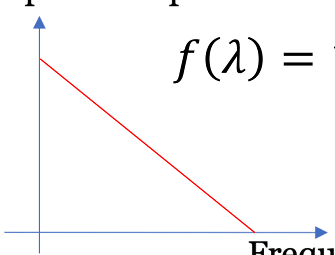

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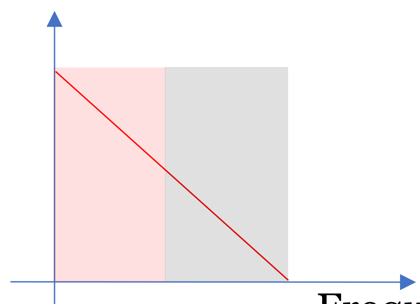

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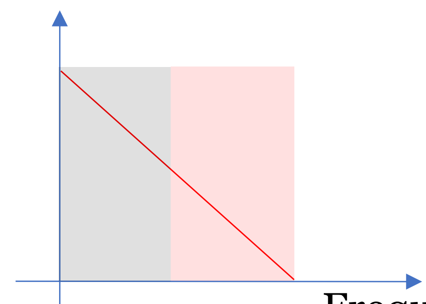

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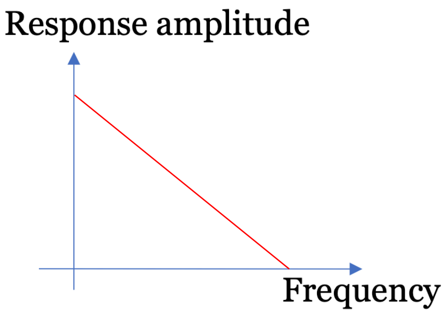
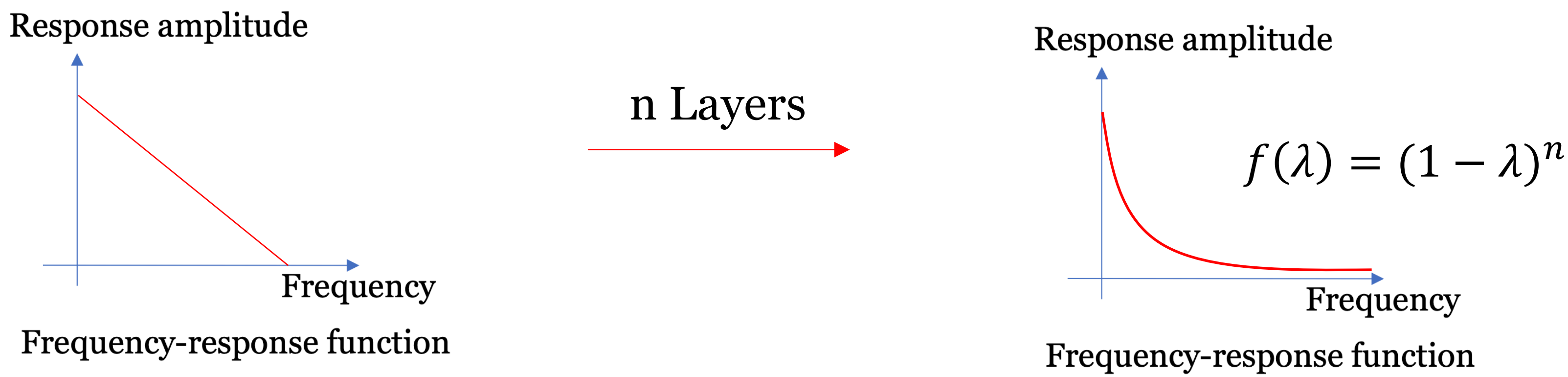


Frequency-response function

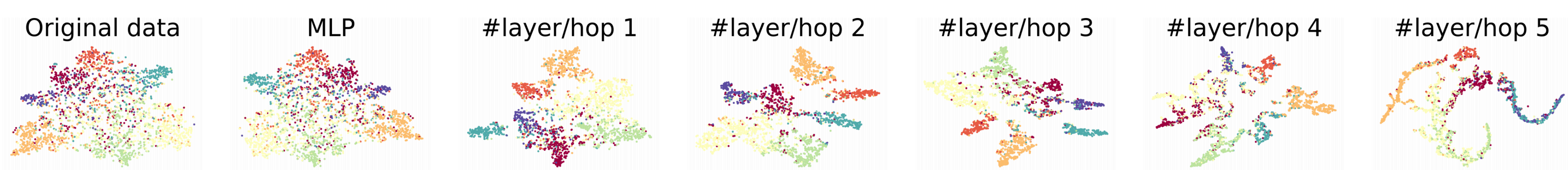
Problem to be tackled: the frequency response function should be **learnable** and **adaptively adjust** itself to capture useful information.

Existing Problems: Over-smoothing

Such fixed filter would greatly reduce most high-frequency components, i.e., making all nodes to be similar to each other.



Node embeddings learned from GCN on Cora dataset [Liu et al. 2020]:



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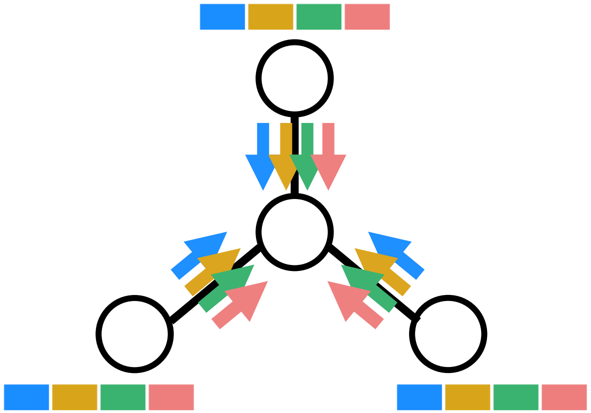
Our Solutions: AdaGNN Layer-wise Illustration

Layer-wise signal filtering operation comparison:

GCN (without learnable matrix)

$$\mathbf{E} = \widetilde{\mathbf{D}}^{-\frac{1}{2}}\widetilde{\mathbf{A}}\widetilde{\mathbf{D}}^{-\frac{1}{2}}\mathbf{X} = \mathbf{X} - \tilde{\mathbf{L}}\mathbf{X}$$



Each channel corresponds to a fixed weight factor for filtering.

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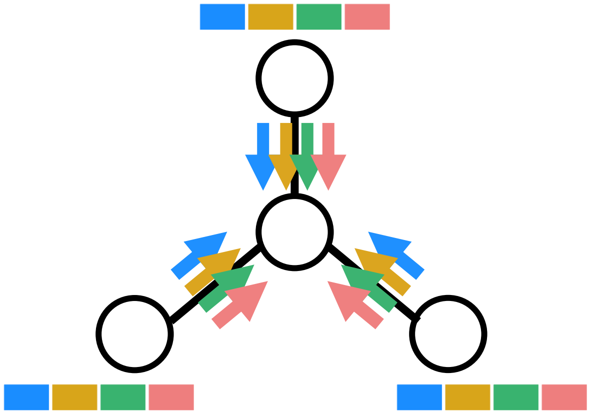

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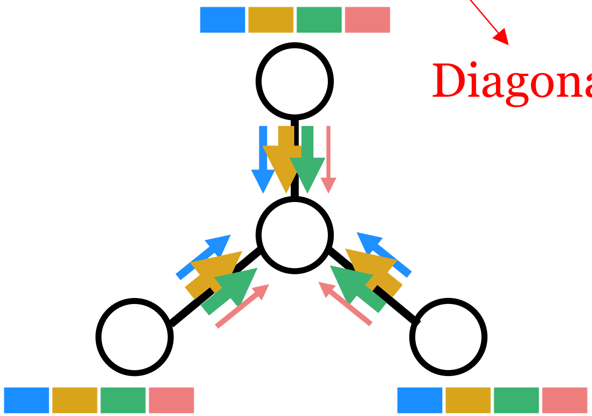
AdaGNN

$$\mathbf{E} = \mathbf{X} - \tilde{\mathbf{L}}\mathbf{X}{\color{red}\mathbf{\Phi}}$$

Diagonal matrix

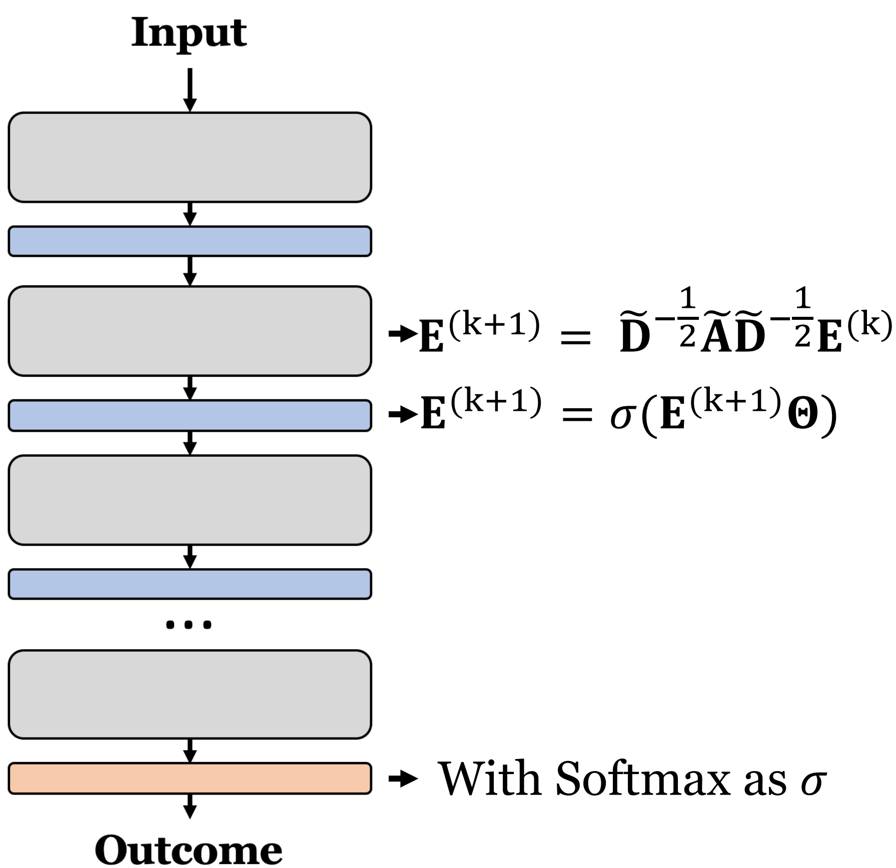


Each channel corresponds to a learnable weight factor ϕ for filtering at each specific layer.

Our Solutions: AdaGNN Model-wise Illustration

Model-wise signal filtering operation comparison:

GCN



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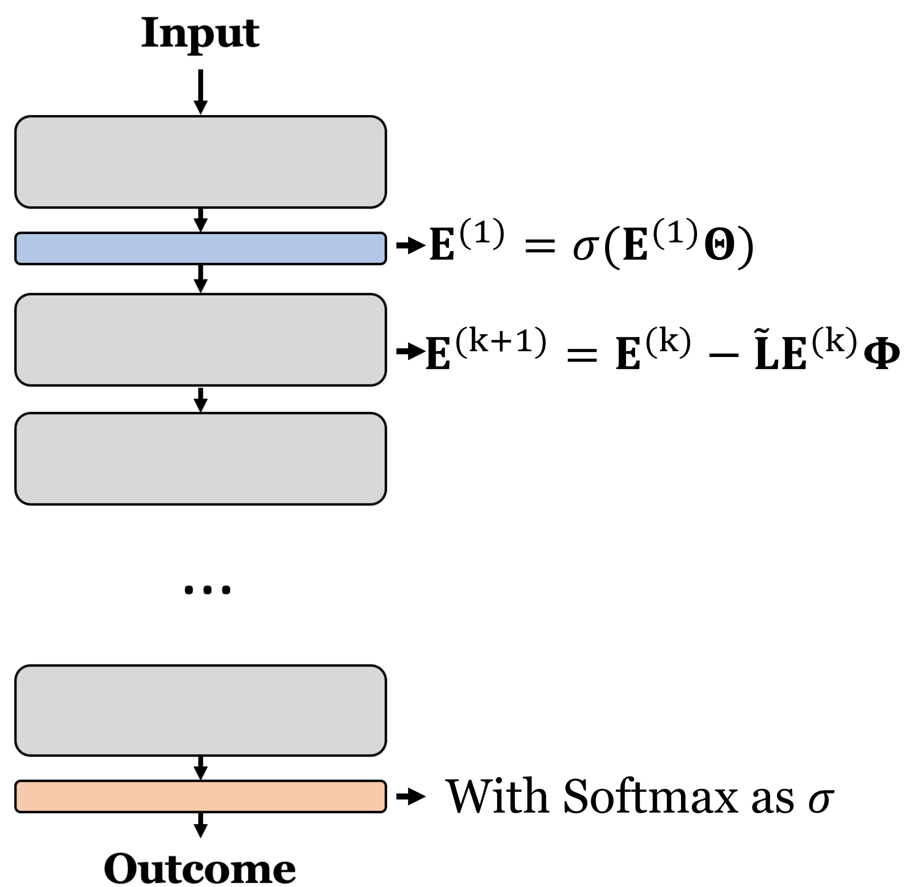

Our Solutions: Learnable Filter in AdaGNN

Question 1: how could this help us to achieve a learnable filter?

	1 Layer	2 Layer	...	n Layer
SGC (without learnable matrix):	$f(\lambda) = 1 - \lambda$	$f(\lambda) = (1-\lambda)^2$		$f(\lambda) = (1-\lambda)^n$
AdaGNN* (one feature dimension):	$f(\lambda) = 1 - \phi_1 \lambda$	$f(\lambda) = \prod_{i=1}^{2}(1-\phi_i\lambda)$		$f(\lambda) = \prod_{i=1}^{n}(1-\phi_i\lambda)$

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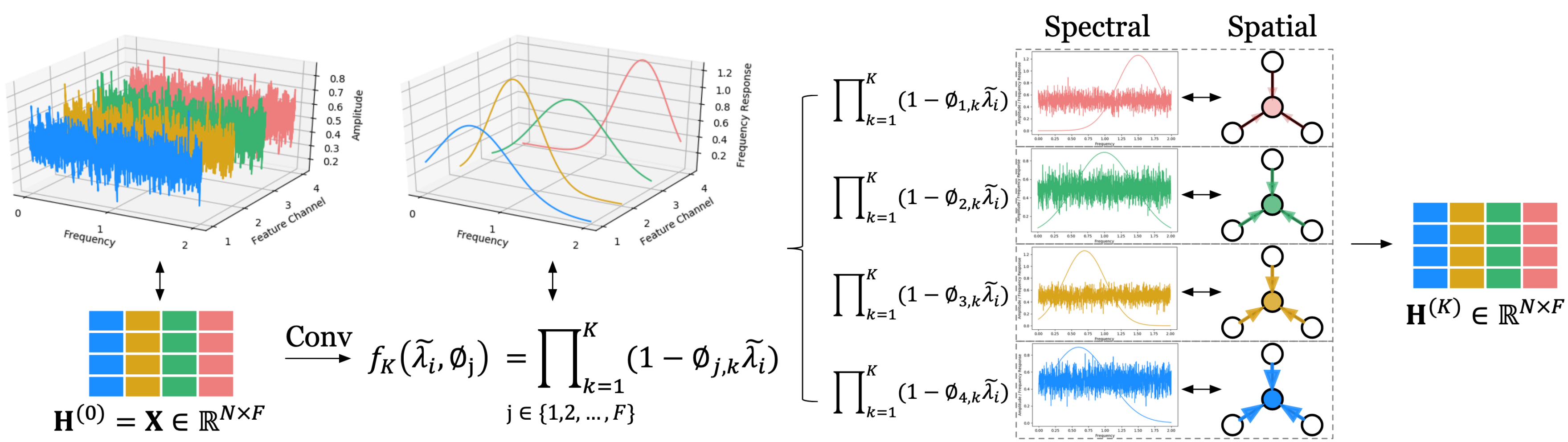
Assume we have four feature dimensions:



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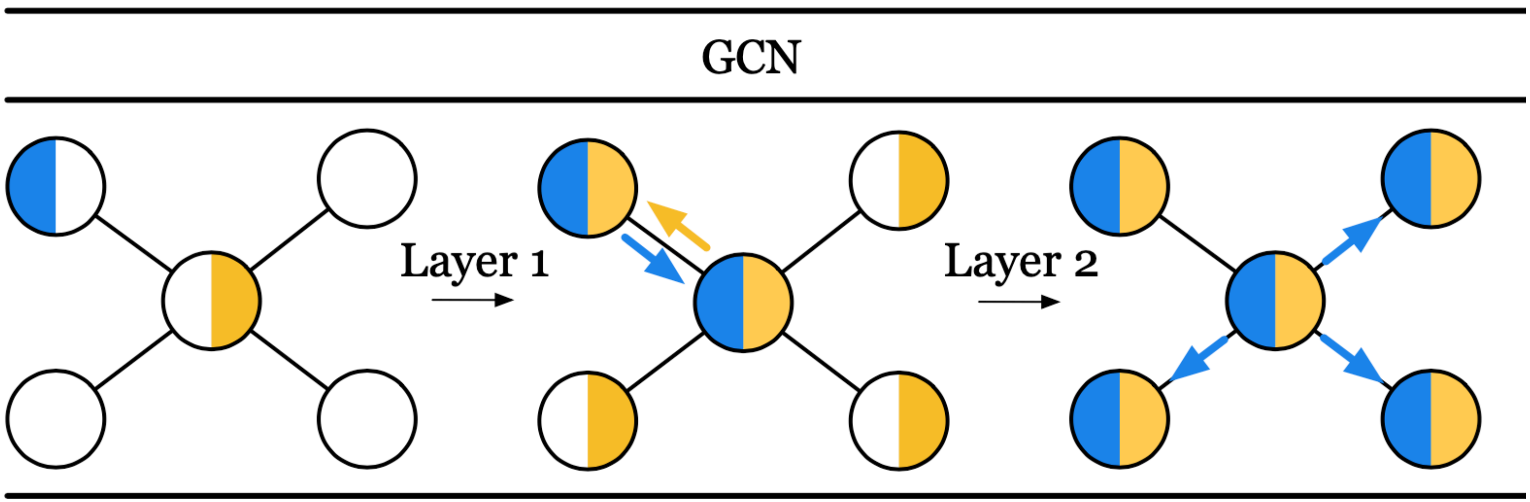
Our Solutions: Toy Example for Over-smoothing Relief

Question 2: how could this help us to relieve over-smoothing?

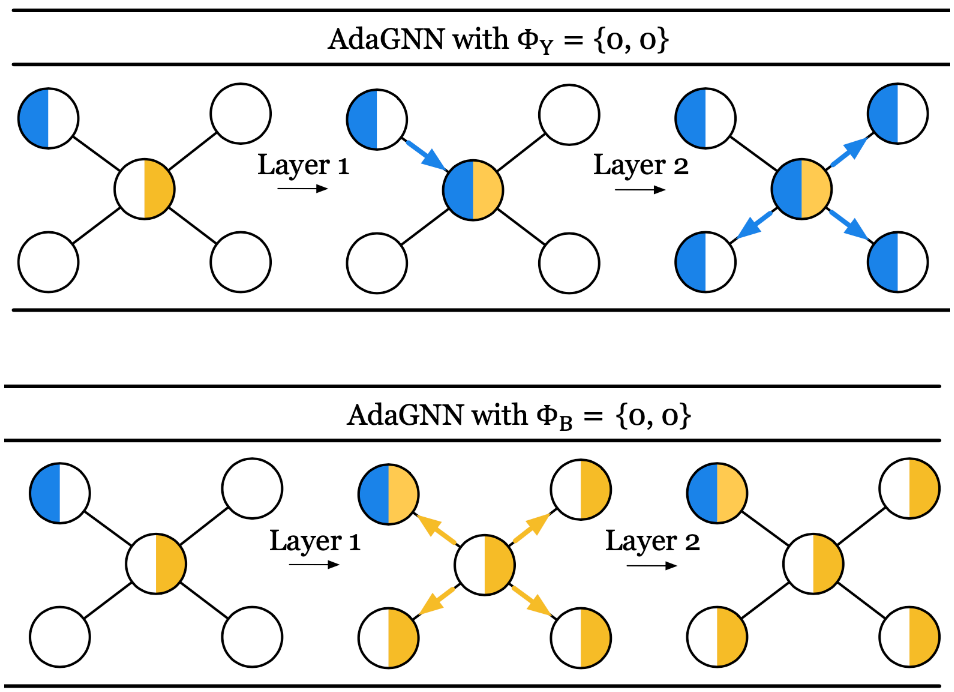


Information is aggregated across different feature dimensions indiscriminately, leading to similar nodes only after 2 layers*.

*In this example, we assume the attribute values can only be binary.

Our Solutions: Toy Example for Over-smoothing Relief

Question 2: how could this help us to relieve over-smoothing?



With learnable ϕs, the embedding of different nodes can be more distinguishable according to their roles after information aggregation.

In AdaGNN, information can be aggregated in a dimension-specific manner*.

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Experiments: General Settings

Downstream tasks:

- Node classification;

Datasets:

- BlogCatalog [Tang et al., 2009] , Flickr [Huang et al., 2017], ACM [Tang et al., 2008], Cora, Citeseer and Pubmed [Sen et al., 2008];

Baselines:

- Three state-of-the-art GNNs including GCN [Kipf et al. 2016], SGC [Wu et al. 2019] and GraphSAGE [Hamilton et al. 2017]; Two recent approaches tackling over-smoothness including Dropedge [Rong et al. 2019] and Pairnorm [Zhao et al. 2019].

	BlogCatalog	Flickr	ACM	Cora	Citeseer	Pubmed
# Nodes	5,196	7,575	16,484	2,708	3,327	19,717
# Edges	173,468	242,146	71,980	5,429	4,732	44,338
# Features	8,189	12,047	8,337	1,433	3,703	500
# Average Degree	66.8	63.9	8.7	4.0	2.8	4.5
# Classes	6	9	9	7	6	3

Experiments: Example Results on BlogCatalog

Our model achieves the **best** performance on prediction accuracy in shallow layer.

Dataset	Model	2 Layer	4 Layer	8 Layer	16 Layer
BlogCatalog	GCN	73.98 ± 0.6%	69.71 ± 0.4%	37.61 ± 2.2%	20.61 ± 1.9%
	GraphSAGE	70.41 ± 0.5%	67.03 ± 0.5%	39.15 ± 1.6%	18.34 ± 3.9%
	SGC	73.97 ± 0.6%	68.94 ± 0.8%	47.94 ± 0.9%	29.02 ± 1.7%
	DropEdge-GCN	74.17 ± 0.7%	70.96 ± 1.3%	60.51 ± 2.4%	51.88 ± 0.8%
	Pairnorm-GCN-SI	67.32 ± 0.7%	63.61 ± 0.9%	65.04 ± 0.6%	67.51 ± 0.4%
	Pairnorm-GCN-SCS	71.67 ± 0.3%	67.01 ± 0.2%	69.30 ± 0.7%	69.75 ± 1.2%
	AdaGNN-R	**86.80 ± 0.3%**	**87.04 ± 0.2%**	**86.68 ± 0.1%**	**86.44 ± 0.5%**
	AdaGNN-S	**88.50 ± 0.2%**	**88.79 ± 0.2%**	**88.81 ± 0.1%**	**88.19 ± 0.2%**

AdaGNN-R: model with asymmetrically normalized $\tilde{\mathbf{L}}$;
AdaGNN-S: model with symmetrically normalized $\tilde{\mathbf{L}}$;

Experiments: Example Results on BlogCatalog

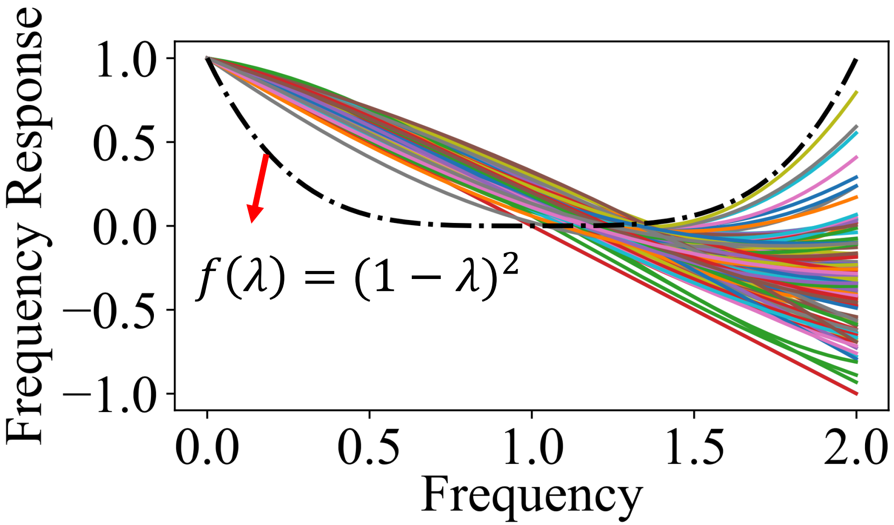
In deeper layers, our model not only achieves the best performance, but also greatly **relieves over-smoothness**.

Dataset	Model	2 Layer	4 Layer	8 Layer	16 Layer
BlogCatalog	GCN	73.98 ± 0.6%	69.71 ± 0.4%	37.61 ± 2.2%	20.61 ± 1.9%
	GraphSAGE	70.41 ± 0.5%	67.03 ± 0.5%	39.15 ± 1.6%	18.34 ± 3.9%
	SGC	73.97 ± 0.6%	68.94 ± 0.8%	47.94 ± 0.9%	29.02 ± 1.7%
	DropEdge-GCN	74.17 ± 0.7%	70.96 ± 1.3%	60.51 ± 2.4%	51.88 ± 0.8%
	Pairnorm-GCN-SI	67.32 ± 0.7%	63.61 ± 0.9%	65.04 ± 0.6%	67.51 ± 0.4%
	Pairnorm-GCN-SCS	71.67 ± 0.3%	67.01 ± 0.2%	69.30 ± 0.7%	69.75 ± 1.2%
	AdaGNN-R	**86.80 ± 0.3%**	**87.04 ± 0.2%**	**86.68 ± 0.1%**	**86.44 ± 0.5%**
	AdaGNN-S	**88.50 ± 0.2%**	**88.79 ± 0.2%**	**88.81 ± 0.1%**	**88.19 ± 0.2%**

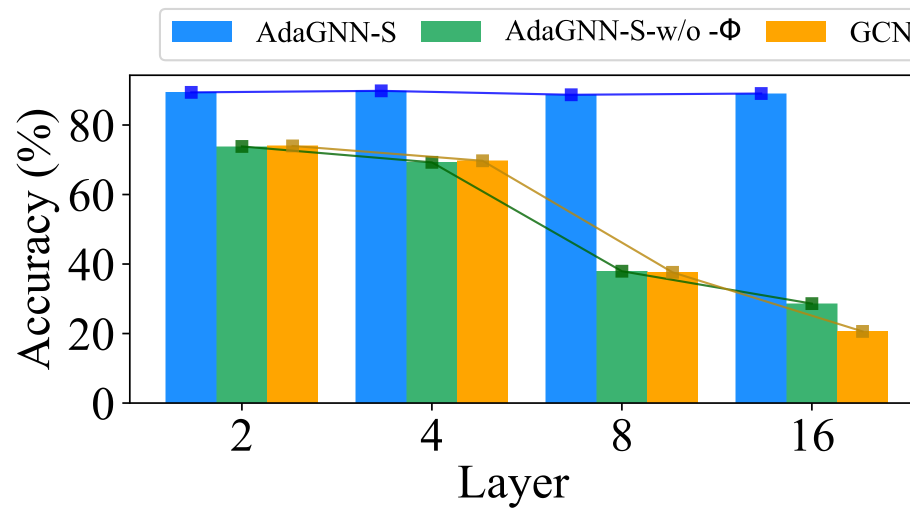
AdaGNN-R: model with asymmetrically normalized $\tilde{\mathbf{L}}$;
AdaGNN-S: model with symmetrically normalized $\tilde{\mathbf{L}}$;

Experiments: Ablation Study

Ablation study with AdaGNN-S as an example:



An visualization of the learned filters across different feature dimension of AdaGNN-S on Flickr dataset.



Model ablation study of AdaGNN-S on BlogCatalog.

Conclusion

- AdaGNN **adaptively** learns the smoothness of each feature dimension, and it achieves a **learnable filter** after multiple layers are stacked together.

- The learnable filter contributes to the **performance superiority** and **over-smoothing relief**.

Overview

Background Introduction

Previous Works

Existing Problems & Challenges

Our Solutions

Experiments & Conclusion

Future Works

Future works

- Fairness issue in spectral GNNs.
- Spectral GNNs with better localized explainability.
- GNNs with learnable and more flexible filter.

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The End

Thanks for listening!