Analyzing the Expressive Power of Graph Neural Networks in a Spectral Perspective



Contributions

- Bridging the gap between spectral and spatial domains in GNN by demonstrating the equivalence of graph convolution processes.
- Propose a new general framework and taxonomy for GNNs.
- Provide theoretical and empirical spectral analysis of GNN models.

Introduction

 Universality of the GNN depends on permutational invariance and ability to produce different outputs for non-isomorphic graphs.



- Expressive power of GNNs were evaluated using equivalence of Weisfeiler-Lehman test order so far.
- MPNN is known to be 1-WL equivalent and WL test order does not tell any differences between MPNNs.
- Since GNN can be seen as a signal processing pipeline, analyzing GNN models in a spectral point of view can bring a new perspective on their expressive power.

Spectral and Spatial GNNs

• **Spectral GNN:** Relies on eigendecomposition of graph Laplacian:

$$H_j^{(l+1)} = \sigma \left(\sum_{i=1}^{f_l} U \mathsf{diag}(F_i^{(l,j)}) U^\top H_i^{(l)} \right)$$

- To overcome drawbacks, trainable weights are parametrized by $F_i^{(l,j)} = B \left[W_{i,j}^{(l,1)}, \dots, W_{i,j}^{(l,s_e)} \right]^\top$
- **Spatial GNN:** Consider an *agg* operator, which aggregates the neighborhood nodes, and an updoperator updates the concerned node as follows:

 $H_{:v}^{(l+1)} = upd\Big(g_0(H_{:v}^{(l)}), agg\Big(g_1(H_{:u}^{(l)}) : u \in \mathcal{N}(v)\Big)\Big)$

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Bridging Spatial and Spectral Domains

• $upd(x,y) = \sigma(x+y)$, agg is a sum of neighbor nodes and g_i applies a linear transformation, Spatial GNN can be written by our general framework by:

$$H^{(l+1)} = \sigma \left(\sum_{s} C^{(s)} H^{(l)} W^{(l,s)}\right)$$

• **Theorem** Spectral GNN parameterized with B of entries $B_{i,j} = \Phi_j(\lambda_i)$ is a particular case of our general framework with the convolution kernel $C^{(s)}$:

$$C^{(s)} = U(\Phi_s(\boldsymbol{\lambda}))U^{\top}.$$

• **Corollary** The frequency profile of a graph convolution support can be defined in spectral domain by:

$$\Phi_s(\boldsymbol{\lambda}) = \mathsf{diag}^{-1}(U^\top C^{(s)}U).$$

Classification of GNN models and their theoretical frequency responses.

Design Support Type			e Convolution Matrix	Frequency Response	low-
MLP	Spectral	Fixed	C = I	$\Phi(\boldsymbol{\lambda}) = 1$	Resi
GCN	Spatial	Fixed	$C = \tilde{D}^{-0.5} \tilde{A} \tilde{D}^{-0.5}$	$\Phi(\boldsymbol{\lambda}) \approx 1 - \boldsymbol{\lambda}\overline{p}/(\overline{p} + 1)$	
GIN	Spatial	Trainable	$C = A + (1 + \epsilon)I$	$\Phi(\boldsymbol{\lambda}) \approx \overline{p}\left(\frac{1+\epsilon}{\overline{p}} + 1 - \boldsymbol{\lambda}\right)$	
GAT	Spatial	Trainable	$C_{v,u}^{(s)} = e_{v,u} / \sum_{k \in \tilde{\mathcal{N}}(v)} e_{v,k}$	NA	
			$C^{(1)} = I$	$\Phi_1(\boldsymbol{\lambda}) = 1$	
CayleyNet	Spectral	Trainable	$C^{(2r)} = Re(ho(hL)^r)$	$\Phi_{2r}(\boldsymbol{\lambda}) = \cos(r\theta(h\boldsymbol{\lambda}))$	02
			$C^{(2r+1)} = Re(\mathbf{i}\rho(hL)^r)$	$\Phi_{2r+1}(\boldsymbol{\lambda}) = -\sin(r\theta(h\boldsymbol{\lambda}))$	50
			$C^{(1)} = I$	$\Phi_1(\boldsymbol{\lambda}) = 1$	
ChebNet	Spectral	Fixed	$C^{(2)} = 2L/\lambda_{\max} - I$	$\Phi_2(\boldsymbol{\lambda}) = 2\boldsymbol{\lambda}/\lambda_{\max} - 1$	• Bar
			$C^{(s)} = 2C^{(2)}C^{(s-1)} - C^{(s-1)}$	$\Phi^{-2)} \Phi_s(\boldsymbol{\lambda}) = 2\Phi_2(\boldsymbol{\lambda})\Phi_{s-1}(\boldsymbol{\lambda}) - \Phi_{s-2}(\boldsymbol{\lambda})$	acco

ChebNet and CayleyNet Freq. Res.





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New Taxonomy of GNN

• **Definition 1:** A **Trainable-support** is a Graph Convolution Support $C^{(s)}$ with at least one trainable parameter that can be tuned during training. If $C^{(s)}$ has no trainable parameters, *i.e.* when the supports are pre-designed, it is called a *fixed-support* graph convolution.

• **Definition 2: Spectral-designed** graph convolution refers to a convolution where supports are written as a function of eigenvalues ($\Phi_s(\boldsymbol{\lambda})$) and eigenvectors (U) of the corresponding graph Laplacian. Thus, each convolution support $C^{(s)}$ has the same frequency response $\Phi_s(\boldsymbol{\lambda})$ over different graphs. Convolution out of this definition is called **spatial-designed** graph convolution.





• Spatial designs are nothing but just low-pass filters! • Spectral designs cover the spectrum well but they do not have band specific filters.



Conclusion of Spectral Analysis

Experimental Results

• **2DGrid Graph** is a node regression problem for -pass, band-pass and high-pass filtered image. ults are in sum of squared error.



ndPass Graph is a binary classification problem ording to frequency that the graph signal carries. MLP GCN GIN GAT ChebNet

Accuracy 50 77.90 87.60 85.30 98.2 0.69 0.454 0.273 0.324 0.062 Loss

• Mnist-75 is a graph classification problem. It is a superpixel graph version of MNIST dataset.

> MLP GCN GIN GAT CayleyNet ChebNet Accuracy 25.10 52.98 75.23 82.73 90.31 92.08

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