Stability of Graph Neural Networks to Relative Perturbations

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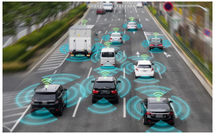
- Graphs are models of signal structure ⇒ Network data ⇒ Leverage in learning from network data

Robot coordination

Smart grids

Remote sensing



Traffic coordination

- Graphs are models of signal structure $\Rightarrow$ Network data $\Rightarrow$ Leverage in learning from network data

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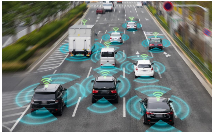

Traffic coordination

- Scalability $\Rightarrow$ Process data from arbitrarily large networks
- Exploit data structure, local information $\Rightarrow$ Fast training and moderate dataset size
- Distributed computations $\Rightarrow$ Efficient implementation

- **Graph Neural Networks**
  - $\Rightarrow$ Graph Signal Processing $\Rightarrow$ Mathematical framework
  - $\Rightarrow$ Graph convolutions $\Rightarrow$ Local, distributed $\Rightarrow$ Generalize time convolutions

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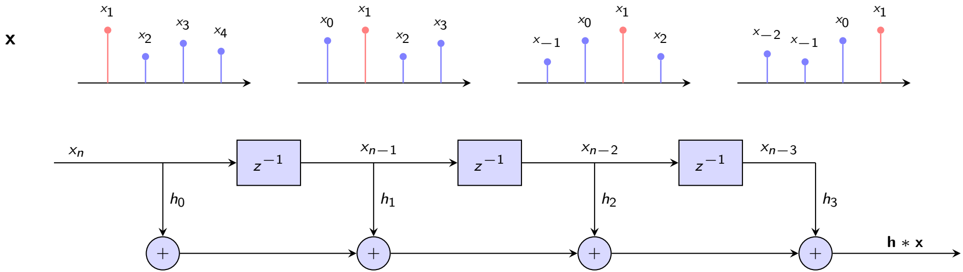
Stability to Perturbations

A small change in the graph support causes a small change in the output of the GNN

Outline

- Graph convolution $\Rightarrow$ Linear combination of shifted versions of the signal $\mathbf{x}$

$$\mathbf{x} * \mathbf{h} = \sum_{k=0}^{K-1} h_k x_{n-k}$$



Gama, Marques, Leus, Ribeiro, "Convolutional Graph Neural Networks", Asilomar, 2019.

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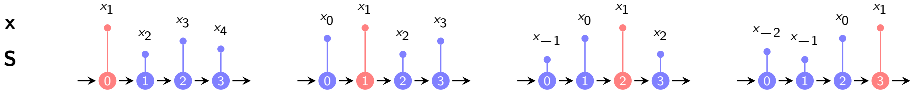
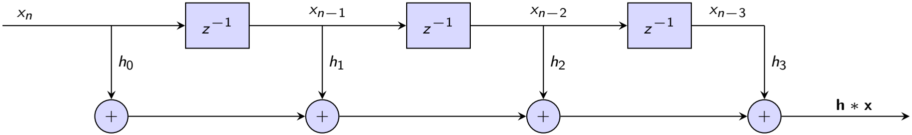
- Notion of shift $\mathbf{S}$ $\Rightarrow$ Matrix description of graph (adjacency, Laplacian)

$$\begin{bmatrix} & \vdots & \vdots & \vdots & \\ \cdots & 0 & 0 & 0 & \cdots \\ \cdots & 1 & 0 & 0 & \cdots \\ \cdots & 0 & 1 & 0 & \cdots \\ \cdots & 0 & 0 & 1 & \cdots \\ & \vdots & \vdots & \vdots & \end{bmatrix}$$





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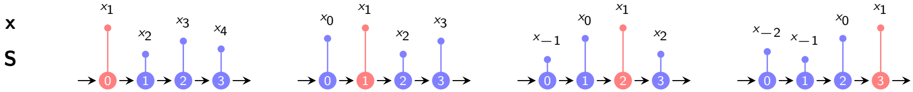

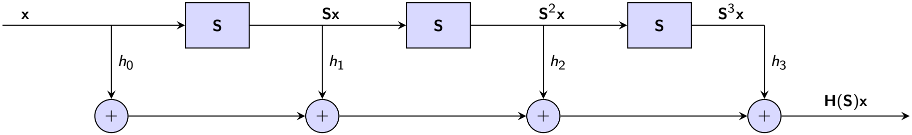

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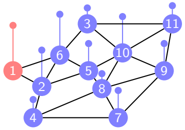
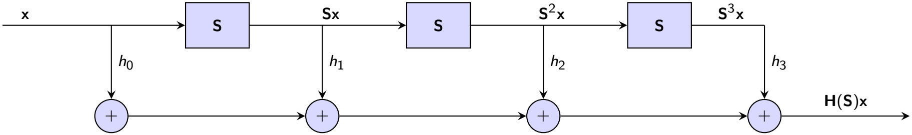
$(\mathbf{x}; \mathbf{S})$





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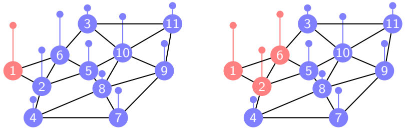

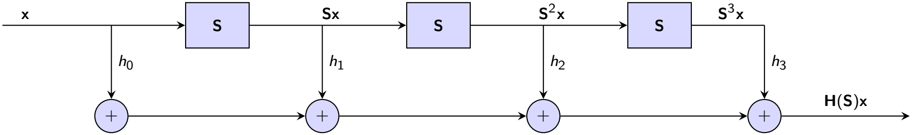

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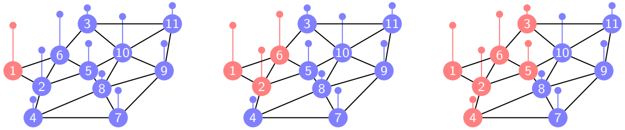

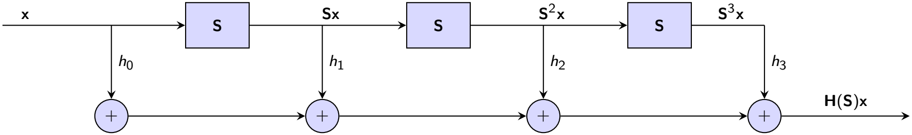

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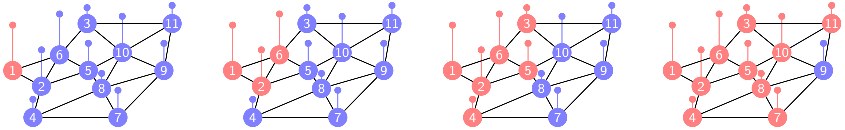

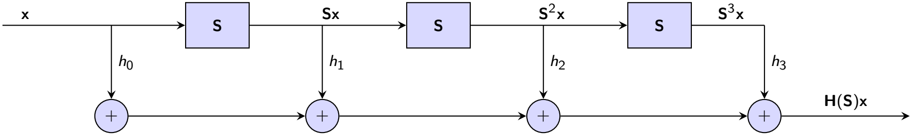

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Graph Convolutions

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- Notion of shift $\mathbf{S}$ $\Rightarrow$ Matrix description of graph (adjacency, Laplacian)
- Linear combination of neighboring signal $\Rightarrow$ Local operation

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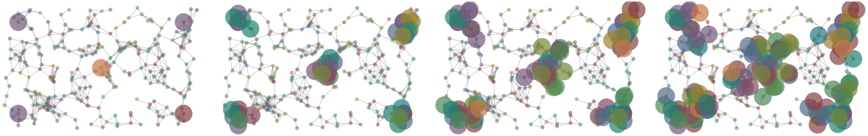

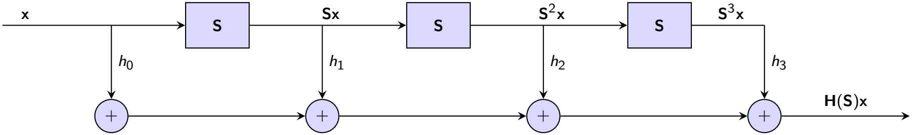

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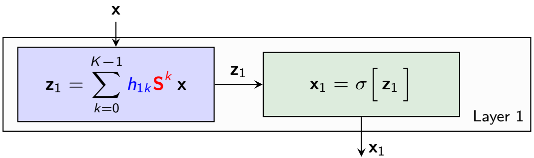
- Cascade of L layers
  - $\Rightarrow$ Graph convolutions with filters $\mathcal{H} = \{\mathbf{h}_\ell\}$
  - $\Rightarrow$ Pointwise nonlinearity (activation functions)



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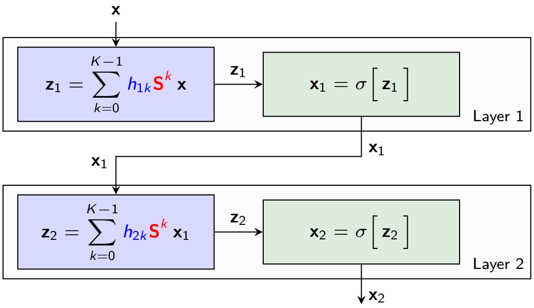

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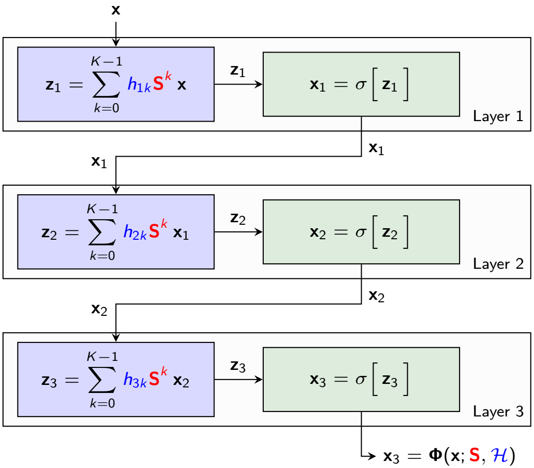
  - $\Rightarrow$ Learn filter taps $\mathcal{H}$ from training data
  - $\Rightarrow$ Also depends on the graph $\mathbf{S}$



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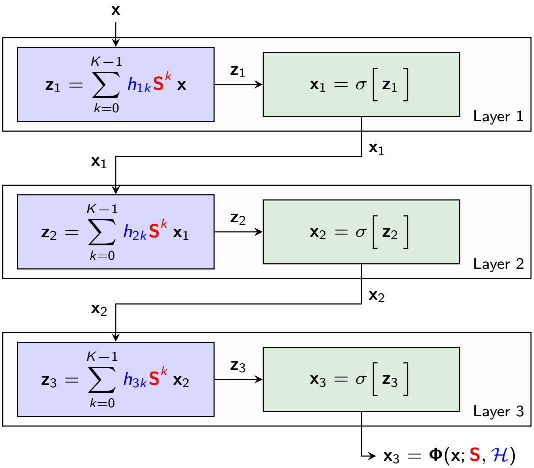
  - $\Rightarrow$ Learn filter taps $\mathcal{H}$ from training data
  - $\Rightarrow$ Also depends on the graph $\mathbf{S}$
- Nonlinear mapping $\mathbf{\Phi}(\mathbf{x}; \mathbf{S}, \mathcal{H})$
  - $\Rightarrow$ Exploit underlying graph structure $\mathbf{S}$
  - $\Rightarrow$ Local information
  - $\Rightarrow$ Distributed implementation



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- Time convolutions are intuitive. Graph convolutions not so much.
  $\Rightarrow$ Local information, efficient implementation (distributed)
- CNNs are good at machine learning $\Rightarrow$ Translation equivariant, stable [Mallat '12]
- Permutation equivariance $\Rightarrow$ Exploit internal symmetries of the graph
- Stability to graph perturbations $\Rightarrow$ Similar graphs yield similar outputs
- Permutation Equivariance + Stablity $\Rightarrow$ Scalability and transferability

- Consider the graph convolution operator $\mathbf{H}(\mathbf{S})\mathbf{x} = \sum_{k=0}^{\infty} h_k \mathbf{S}^k \mathbf{x}$
- Depends on filter parameters $\mathbf{h} = \{h_k\}_{k=0}^{\infty}$ and shift operator $\mathbf{S}$; applied to the input signal $\mathbf{x}$

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Theorem

Graph convolutions are equivariant to permutations. For graphs with permuted shift operators $\hat{\mathbf{S}} = \mathbf{P}^{\mathsf{T}}\mathbf{S}\mathbf{P}$ and permuted graph signals $\hat{\mathbf{x}} = \mathbf{P}^{\mathsf{T}}\mathbf{x}$ it holds

$$\mathbf{H}(\hat{\mathbf{S}})\hat{\mathbf{x}} = \mathbf{P}^{\mathsf{T}}\mathbf{H}(\mathbf{S})\mathbf{x}$$

Proof $\Rightarrow$ $\mathbf{H}(\hat{\mathbf{S}})\hat{\mathbf{x}} = \sum_{k=0}^{\infty} h_k \, \hat{\mathbf{S}}^k \hat{\mathbf{x}} = \sum_{k=0}^{\infty} h_k \, (\mathbf{P}^{\mathsf{T}}\mathbf{S}\mathbf{P})^k \mathbf{P}^{\mathsf{T}}\mathbf{x} = \mathbf{P}^{\mathsf{T}} \left(\sum_{k=0}^{\infty} h_k \, \mathbf{S}^k \mathbf{x} \right) = \mathbf{P}^{\mathsf{T}}\mathbf{H}(\mathbf{S})\mathbf{x}$

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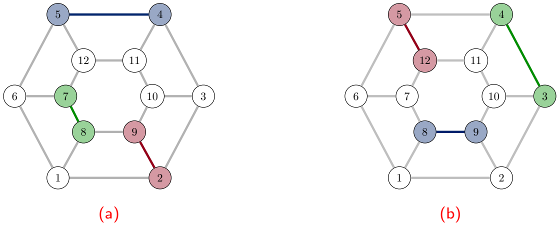
- GNN $\Rightarrow$ Graph convolution + Pointwise nonlinearity $\Rightarrow$ Pointwise does not mix node values
  $\Rightarrow$ GNN retains permutation equivariance $\Rightarrow$ $\mathbf{\Phi}(\hat{\mathbf{x}}; \hat{\mathbf{S}}, \mathcal{H}) = \mathbf{P}^\mathsf{T}\mathbf{\Phi}(\mathbf{x}; \mathbf{S}, \mathcal{H})$
- Signal processing with graph neural networks is independent of labeling

- Invariance to node relabelings allows GNNs to exploit internal symmetries of graph signals
- Although different, signals on (a) and (b) are permutations of one other
  $\Rightarrow$ Permutation equivariance means that the GNN can learn to classify (b) from seeing (a)



- Permutation Equivariance is not a good idea in all problems $\Rightarrow$ Edge-Variant GNNs

Isufi, **Gama**, Ribeiro, "EdgeNets: Edge Varying Graph Neural Networks", arXiv:2001.07620, 2020

Equivariance to Permutations is a Property of Graph Filters

- Permutation equivariance is a property of graph convolutions inherited to GNNs
  - $\Rightarrow$ Exploits data structure (internal symmetries of the graph)
- Why choose GNNs over graph convolutions?
  - $\Rightarrow$ Q1: What is good about pointwise nonlinearities?
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- These questions can be answered with an analysis in the **spectral domain**

- Graph convolution is a polynomial on the shift operator $\Rightarrow \mathbf{y} = \sum_{k=0}^{\infty} h_k \mathbf{S}^k \mathbf{x}$

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- Decompose operator as $\mathbf{S} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^{\mathsf{H}}$ to write the spectral representation of the graph convolution

$$\mathbf{V}^{\mathsf{H}}\mathbf{y} = \mathbf{V}^{\mathsf{H}} \sum_{k=0}^{\infty} h_k (\mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^{\mathsf{H}})^k \mathbf{x} \quad \Rightarrow \quad \tilde{\mathbf{y}} = \sum_{k=0}^{\infty} h_k \boldsymbol{\Lambda}^k \tilde{\mathbf{x}}$$

- where we have used the graph Fourier transform (GFT) definitions $\tilde{\mathbf{x}} = \mathbf{V}^{\mathsf{H}}\mathbf{x}$ and $\tilde{\mathbf{y}} = \mathbf{V}^{\mathsf{H}}\mathbf{y}$

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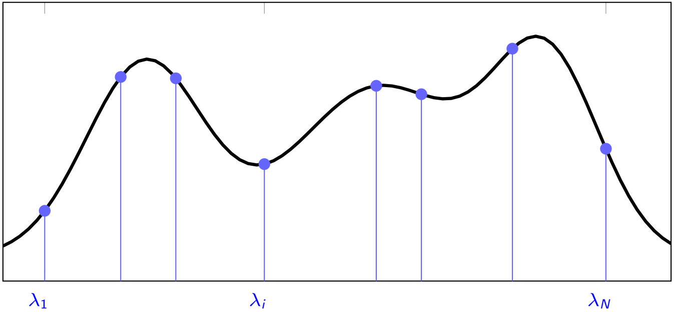
- where we have used the graph Fourier transform (GFT) definitions $\tilde{\mathbf{x}} = \mathbf{V}^{\mathsf{H}}\mathbf{x}$ and $\tilde{\mathbf{y}} = \mathbf{V}^{\mathsf{H}}\mathbf{y}$
- Graph convolution is a pointwise operation in the spectral domain

$$\tilde{y}_i \;=\; \tilde{h}(\lambda_i) \cdot \tilde{x}_i$$

$\Rightarrow$ Determined by the (graph) frequency response $\Rightarrow \sum_{k=0}^{\infty} h_k \lambda_i^k = \tilde{h}(\lambda_i)$

- We can reinterpret the frequency response as a polynomial on continuous λ $\Rightarrow \tilde{h}(\lambda) = \sum_{k=0}^{\infty} h_k \lambda^k$



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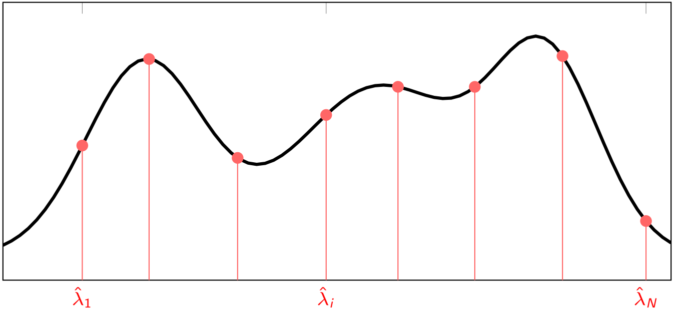

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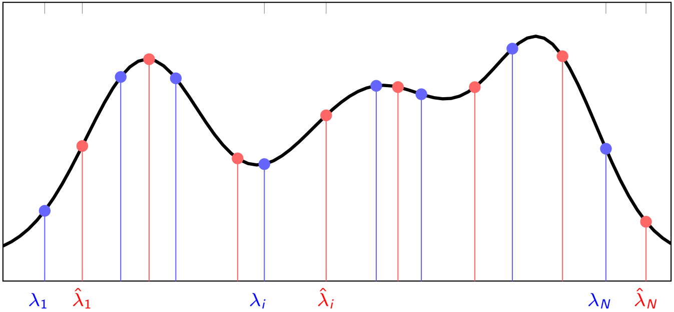
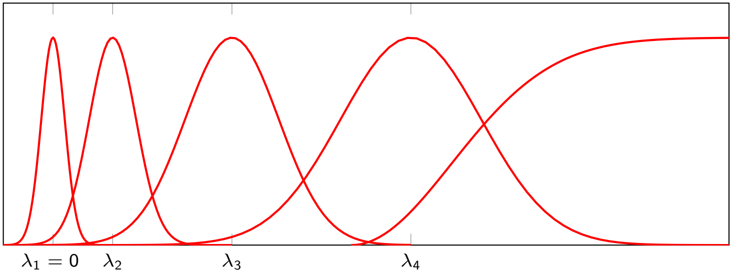
- We can reinterpret the frequency response as a polynomial on continuous λ $\Rightarrow \tilde{h}(\lambda) = \sum_{k=0}^{\infty} h_k \lambda^k$



- Frequency response is the same no matter the graph $\Rightarrow$ It's instantiated on its particular spectrum

- Let $h(\lambda)$ be the frequency response of filter $\mathbf{H}$. We say $\mathbf{H}$ is integral Lipschitz if $|\lambda h'(\lambda)| \leq C$



- Integral Lipschitz filters have to be wide for large λ $\Rightarrow$ They cannot discriminate
- But they can be thin for low λ $\Rightarrow$ They can discriminate. Arbitrarily discriminate

- Relative distance between $\mathbf{S}$ and $\hat{\mathbf{S}}$ $\Rightarrow$ Smallest matrix $\mathbf{E}$ that maps $\mathbf{S}$ into a permutation of $\hat{\mathbf{S}}$

$$\mathcal{E} = \left\{ \mathbf{E} : \mathbf{P}^{\mathsf{T}} \hat{\mathbf{S}} \mathbf{P} = \mathbf{S} + \mathbf{E}^{\mathsf{T}} \mathbf{S} + \mathbf{S} \mathbf{E} \right\} \quad \Rightarrow \quad d(\mathbf{S}, \hat{\mathbf{S}}) = \min_{\mathbf{E} \in \mathcal{E}} \| \mathbf{E} \| \leq \frac{\| \hat{\mathbf{S}} - \mathbf{S} \|}{\| \mathbf{S} \|}$$

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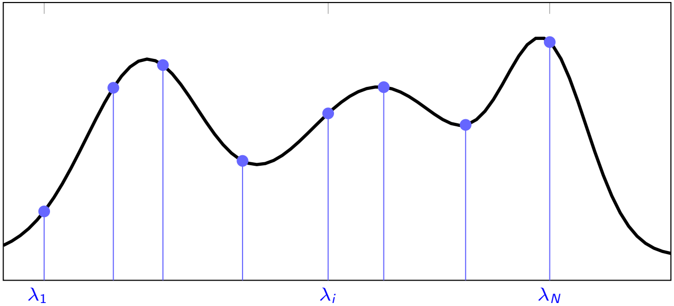
Theorem

Consider a GNN with L layers having integral Lipschitz filter $\mathbf{H}_\ell$ with constant C. Graphs $\mathbf{S}$ and $\hat{\mathbf{S}}$ satisfy $d(\mathbf{S}, \hat{\mathbf{S}}) \leq \epsilon/2$. The matrix $\mathbf{E}$ that achieves minimum distance satisfies $\|\mathbf{E}/\|\mathbf{E}\| - \mathbf{I}\| \leq \varepsilon$. It holds that for all signals $\mathbf{x}$

$$\min_{\mathbf{P} \in \mathcal{P}} \|\Phi(\mathbf{x}; \hat{\mathbf{S}}, \mathcal{H}) - \mathbf{P}^{\mathsf{T}} \Phi(\mathbf{x}; \mathbf{S}, \mathcal{H})\| \leq CL\, \varepsilon + \mathcal{O}(\varepsilon^2)$$

- GNNs can be made stable to graph perturbations if filters are integral Lipschitz

- The GNN stability theorem is elementary to prove for an edge dilation $\Rightarrow \hat{\mathbf{S}} = (1+\varepsilon)\mathbf{S}$
- An edge dilation just produces a spectrum dilation $\Rightarrow \hat{\lambda}_i = (1+\varepsilon)\lambda_i$, $\mathbf{E} = (\varepsilon/2)\mathbf{I}$



- Small deformations may result in large filter variations for large λ if filter is not integral Lipschitz

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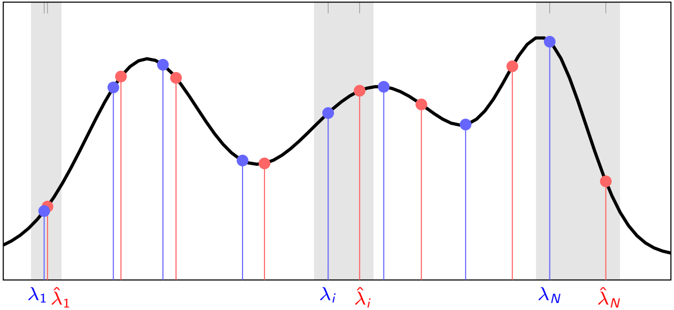

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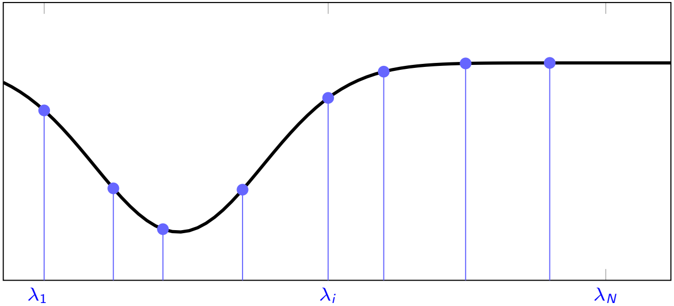

- Integral Lipschitz is always stable $\Rightarrow$ Eigenvalue does not move or filter does not move

Proof of Stability Theorem

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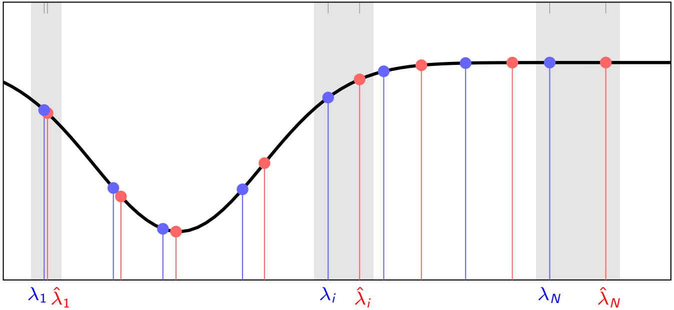
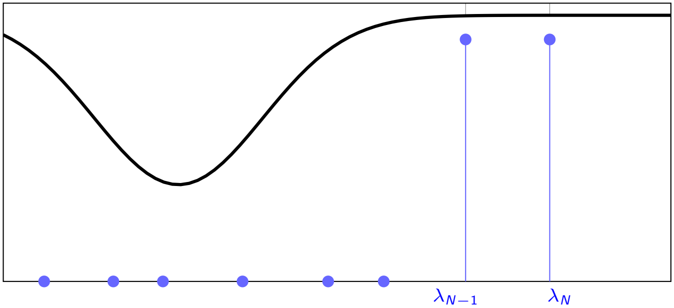


- Integral Lipschitz is always stable $\Rightarrow$ Eigenvalue does not move or filter does not move

- Q2: What is wrong with linear graph convolutions?
- Cannot be simultaneously stable to deformations and discriminate features at large eigenvalues



- Limits their value in machine learning problems where features at large eigenvalues are important

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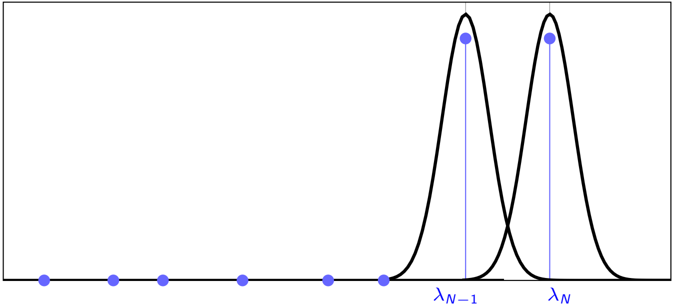

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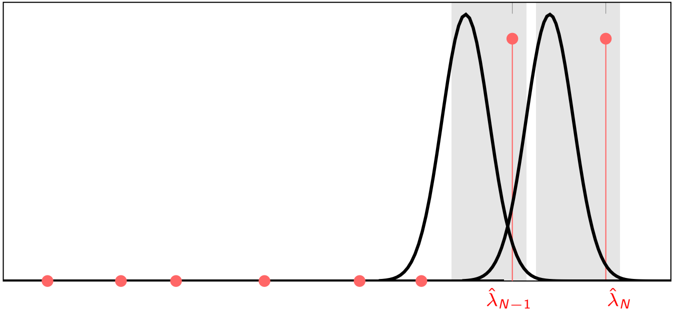

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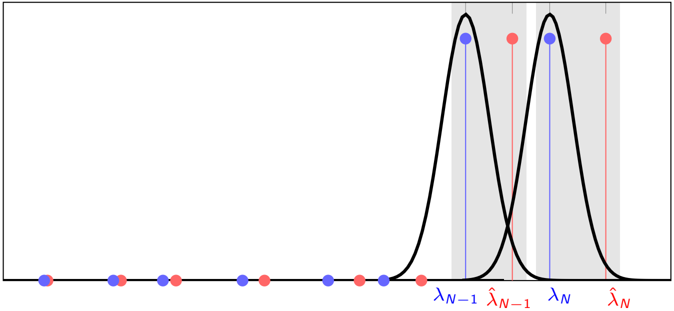
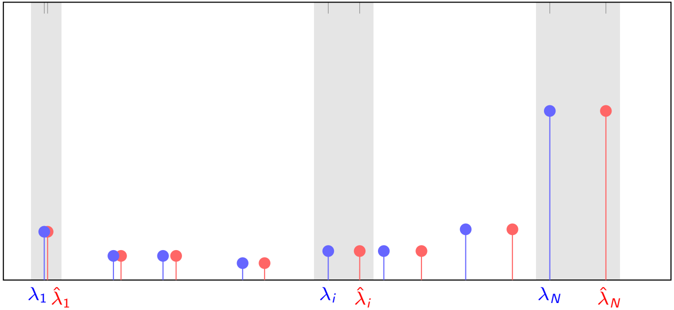


- Limits their value in machine learning problems where features at large eigenvalues are important

- Q1: What is good about pointwise nonlinearities?
- Preserve permutation equivariance while generating low graph frequency components
  $\Rightarrow$ Which we can discriminate with stable filters



Spectrum of rectified graph signal

$$\mathbf{x}_{\text{relu}} = \max(\mathbf{x}, 0)$$

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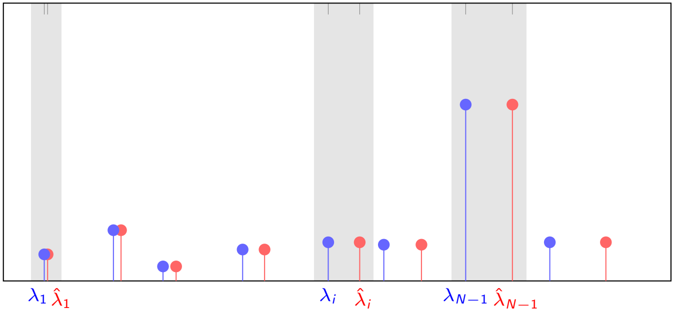

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Nonlinearities Create Low Frequency Components

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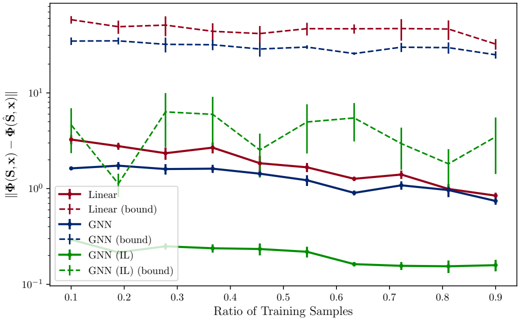
GNNs are **stable** and **selective** information processing architectures

- The nonlinearity demodulates. It creates low frequency content that is stable

Example: Movie Recommendation Systems

- Movie recommendation problem $\Rightarrow$ Each node is a movie, each edge is the rating similarity
- Rating similarities estimated from training set $\Rightarrow$ Changing training set changes graph



- GNN trained with integral Lipschitz filters is more stable to graph estimation errors

Gama, Isufi, Leus, Ribeiro, "Graphs, Convolutions, and Neural Networks", arXiv:2003.03777, 2020

Gama, Tolstaya, Ribeiro, "Graph Neural Networks for Decentralized Controllers", arXiv:2003.10280, 2020

- Successful learning on graphs $\Rightarrow$ Scalability, exploit data structure, distributed implementation
- Graph neural networks (GNNs) $\Rightarrow$ Graph convolutions followed by pointwise nonlinearities
- GNNs are permutation equivariant and stable to changes in the graph $\Rightarrow$ Scale, transfer
- Graph convolutions are either stable or selective, but cannot be both
- Nonlinearities $\Rightarrow$ GNNs are both **stable** and **selective** information processing architectures
- Movie recommendation $\Rightarrow$ Stable to estimation errors in the rating similarity

Journal version:

Gama, Bruna, Ribeiro, "Stability Properties of Graph Neural Networks", arXiv:1905.04497, 2020.

Thank You!