

Additive Perturbations of Graph Filters

- ▶ We define additive perturbations of the graph support

- ▶ Graph filter $\mathbf{H}(\mathbf{S})$ is a polynomial on **shift operator \mathbf{S}** with coefficients h_k . Outputs given by

$$\mathbf{H}(\mathbf{S}) \mathbf{x} = \sum_{k=0}^{K-1} h_k \mathbf{S}^k \mathbf{x}$$

- ▶ Perturbations of the **input** \Rightarrow The filter is **linear in \mathbf{x}** . Scale error by filter's norm.
- ▶ Perturbations of the **coefficients** \Rightarrow Filter is **linear in h_k** . Plus, h_k is a **design parameter**.
- ▶ **Perturbations** of the shift operator \mathbf{S} \Rightarrow It is **not easy** (nonlinear). And it is **necessary**.
 - \Rightarrow The graph is **estimated** (recommendation systems). The graph **changes** (distributed systems)
 - \Rightarrow **Quasi-symmetries** in graphs that are quasi-invariant to permutations

- ▶ Apply the **same filter \mathbf{h}** to the **same signal \mathbf{x}** on **different graphs** shift operators **\mathbf{S}** and **$\hat{\mathbf{S}}$**

$$\mathbf{H}(\mathbf{S}) \mathbf{x} = \sum_{k=0}^{K-1} h_k \mathbf{S}^k \mathbf{x} \qquad \mathbf{H}(\hat{\mathbf{S}}) \mathbf{x} = \sum_{k=0}^{K-1} h_k \hat{\mathbf{S}}^k \mathbf{x}$$

- ▶ Filter **$\mathbf{H}(\mathbf{S}) \mathbf{x}$** \Rightarrow Coefficients **h_k** . Input signal **\mathbf{x}** . Instantiated on shift **\mathbf{S}**
- ▶ Filter **$\mathbf{H}(\hat{\mathbf{S}}) \hat{\mathbf{x}}$** \Rightarrow **Same** Coefficients **h_k** . **Same** Input signal **\mathbf{x}** . Instantiated on **perturbed** shift **$\hat{\mathbf{S}}$**
- ▶ We investigated scalings **$\hat{\mathbf{S}} = (1 + \epsilon)\mathbf{S}$** are an example. But we are after more generic models.

- ▶ Additive perturbation model $\Rightarrow \hat{\mathbf{S}} = \mathbf{S} + \mathbf{E}$.
- ▶ Error matrix $\mathbf{E} = \hat{\mathbf{S}} - \mathbf{S}$ exists for any pair $\mathbf{S}, \hat{\mathbf{S}}$. \Rightarrow It's norm $\|\mathbf{E}\|$ quantifies their difference
- ▶ A flaw \Rightarrow Graphs \mathbf{S} and $\hat{\mathbf{S}} = \mathbf{P}^T \mathbf{S} \mathbf{P}$ are the same (relabeling). Yet we may not have $\|\mathbf{E}\| = 0$.
- ▶ We know better \Rightarrow Operator distances modulo permutation $\|\hat{\mathbf{S}} - \mathbf{S}\|_{\mathcal{P}} = \min_{\mathcal{P}} \|\hat{\mathbf{S}} \mathbf{P}^T - \mathbf{P}^T \mathbf{S}\|$

- ▶ We need a concrete **handle on the error matrix**. Start from set of symmetric error matrices

$$\mathcal{E}(\mathbf{S}, \hat{\mathbf{S}}) = \left\{ \tilde{\mathbf{E}} : \mathbf{P}^T \hat{\mathbf{S}} \mathbf{P} = \mathbf{S} + \tilde{\mathbf{E}}, \quad \mathbf{P} \in \mathcal{P} \right\}$$

- ▶ For each permutation $\mathbf{P} \in \mathcal{P}$ we have a different error matrix $\tilde{\mathbf{E}} = \mathbf{P}^T \hat{\mathbf{S}} \mathbf{P} - \mathbf{S}$ in the set $\mathcal{E}(\mathbf{S}, \hat{\mathbf{S}})$
- ▶ **Error matrix modulo permutation** is the one with smallest norm $\Rightarrow \mathbf{E} = \underset{\tilde{\mathbf{E}} \in \mathcal{E}(\mathbf{S}, \hat{\mathbf{S}})}{\operatorname{argmin}} \|\tilde{\mathbf{E}}\|$
- ▶ Rewrite the distance modulo permutation as $\Rightarrow d(\mathbf{S}, \hat{\mathbf{S}}) = \|\mathbf{E}\| = \min_{\tilde{\mathbf{E}} \in \mathcal{E}(\mathbf{S}, \hat{\mathbf{S}})} \|\tilde{\mathbf{E}}\|$
- ▶ Error norm $\|\mathbf{E}\| = d(\mathbf{S}, \hat{\mathbf{S}})$ measures how far \mathbf{S} and $\hat{\mathbf{S}}$ are from being **permutations of each other**

- ▶ Consider eigenvector decompositions of the shift $\mathbf{S} = \mathbf{V}\Lambda\mathbf{V}^H$ and the error $\mathbf{E} = \mathbf{U}\mathbf{M}\mathbf{U}^H$
- ▶ Define the **eigenvector misalignment** between the shift operator \mathbf{S} and the error matrix \mathbf{E} as

$$\delta = \left(\|\mathbf{U} - \mathbf{V}\| + 1 \right)^2 - 1$$

- ▶ Since \mathbf{U} and \mathbf{V} are unitary matrices $\|\mathbf{U}\| = \|\mathbf{V}\| = 1 \Rightarrow \delta \leq 8 = [(2 + 1)^2 - 1]$

\Rightarrow The eigenvector misalignment δ is never large. It can be small. Depending on the error model.

Stability of Lipschitz Filters to Additive Perturbations

- ▶ We show that Lipschitz filters are stable to additive perturbations of the graph support.

Theorem (Lipschitz Filters are Stable to Additive Perturbations)

Consider **graph filter \mathbf{h}** along with shift operators **\mathbf{S}** and **$\hat{\mathbf{S}}$** having **n nodes**. If it holds that:

(H1) Shift operators **\mathbf{S}** and **$\hat{\mathbf{S}}$** are related by **$\mathbf{P}^T \hat{\mathbf{S}} \mathbf{P} = \mathbf{S} + \mathbf{E}$** with **$\mathbf{P}$** a permutation matrix

(H2) The **error matrix \mathbf{E}** has norm **$\|\mathbf{E}\| = \epsilon$** and **eigenvector misalignment δ** relative to **\mathbf{S}**

(H3) The filter **\mathbf{h}** is **Lipschitz** with constant **C**

Then, the operator distance modulo permutation between filters **$\mathbf{H}(\mathbf{S})$** and **$\mathbf{H}(\hat{\mathbf{S}})$** is bounded by

$$\|\mathbf{H}(\hat{\mathbf{S}}) - \mathbf{H}(\mathbf{S})\|_{\mathcal{P}} \leq C(1 + \delta\sqrt{n})\epsilon + \mathcal{O}(\epsilon^2).$$

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The operator distance modulo permutation between filters $\mathbf{H}(\mathbf{S})$ and $\mathbf{H}(\hat{\mathbf{S}})$ satisfies

$$\|\mathbf{H}(\hat{\mathbf{S}}) - \mathbf{H}(\mathbf{S})\|_{\mathcal{P}} \leq C(1 + \delta\sqrt{n})\epsilon + \mathcal{O}(\epsilon^2).$$

- ▶ If shifts \mathbf{S} and $\hat{\mathbf{S}}$ are ϵ -close the filters $\mathbf{H}(\mathbf{S})$ and $\mathbf{H}(\hat{\mathbf{S}})$ are ϵ -close. Modulo permutation
- ▶ Proportional to the Lipschitz constant of the filter's frequency response. Not integral Lipschitz
- ▶ Proportional to $(1 + \delta\sqrt{n})$. Not great for large graphs. Unless misalignment decreases with n .
- ▶ Growth with n is at most $(1 + 8\sqrt{n}) \geq (1 + \delta\sqrt{n})$. Because $\delta \leq 8$. Not that bad

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- ▶ Filter perturbations are first order **Lipschitz continuous** with respect to the **perturbation's size ϵ**
 - ⇒ With **Lipschitz** constant ⇒ **$C(1 + \delta\sqrt{n})$**
- ▶ Stronger than plain continuity. Which would say “output changes are small if input changes are”

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$$\|\mathbf{H}(\hat{\mathbf{S}}) - \mathbf{H}(\mathbf{S})\|_{\mathcal{P}} \leq C (1 + \delta\sqrt{n}) \epsilon + \mathcal{O}(\epsilon^2).$$

- ▶ Bound is universal for all graphs with a given number of nodes n . Bound depends on:
 - ⇒ A property of the filter's frequency response. The filter's Lipschitz constant C
 - ⇒ And properties of the perturbation \mathbf{E} . The eigenvector misalignment δ and the norm $\|\mathbf{E}\| = \epsilon$
- ▶ There is no constant in the bound that depends on the graph shift operator \mathbf{S} . Save for n .

Theorem (Lipschitz Filters are Stable to Additive Perturbations)

The operator distance modulo permutation between filters $\mathbf{H}(\mathbf{S})$ and $\mathbf{H}(\hat{\mathbf{S}})$ satisfies

$$\|\mathbf{H}(\hat{\mathbf{S}}) - \mathbf{H}(\mathbf{S})\|_{\mathcal{P}} \leq C(1 + \delta\sqrt{n})\epsilon + \mathcal{O}(\epsilon^2).$$

- ▶ The filter's Lipschitz constant C is a parameter that we can affect with judicious filter choice
- ▶ **Discriminability / stability tradeoff.** Larger C improves discriminability at the cost of stability

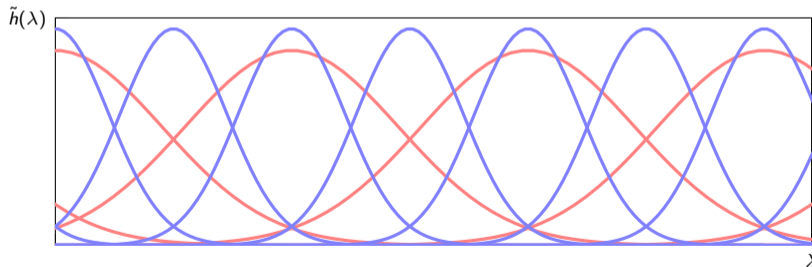
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- ▶ Eigenvector misalignment δ is a **property of the perturbation matrix**. Independent of filter choice
 \Rightarrow **Not very relevant** in studying stability / discriminability tradeoffs of different filters.
- ▶ **Meaningless asymptotically on n** . Don't know much about perturbations in the limit of large n

- ▶ Stability to additive perturbations **requires Lipschitz filters**. Not integral Lipschitz as with scalings
- ▶ Genuine stability / discriminability tradeoff \Rightarrow **Larger C tradeoffs stability for discriminability**
- ▶ We can always discriminate, **regardless of frequency**, if we tolerate enough discriminability.



Relative Perturbations of Graph Filters

- ▶ Proved enticing stability properties with respect to **additive perturbations**. Alas, **not meaningful**
- ▶ We switch focus to **relative perturbations**. Which tie perturbations to the graph structure

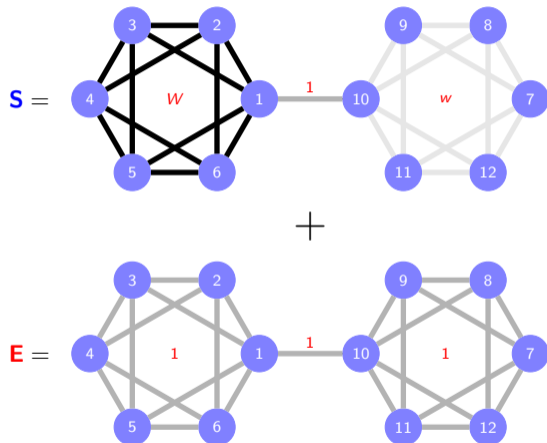
- ▶ Additive perturbations are **not meaningful**

$$P^T \hat{S} P = S + E$$

- ▶ With $w \ll 1 \ll W$.

⇒ Is this perturbation **small or large?**

- ▶ Edges with small weights w can change a lot because other edges have large weights W



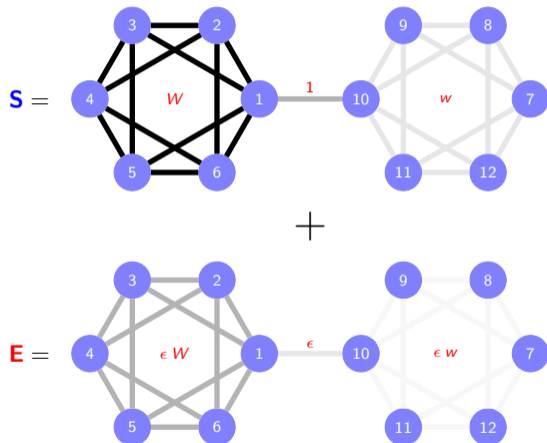
- ▶ Relative perturbations are **more meaningful**

$$P^T \hat{S} P = S + E = S + \epsilon I S$$

- ▶ With $w \ll 1 \ll W$ and $\epsilon \ll 1$

⇒ Is this perturbation **small or large?**

- ▶ **It's small.** Edges with small weights change little. Edges with large weights change more



▶ **Relative** perturbation model $\Rightarrow \hat{\mathbf{S}} = \mathbf{S} + \mathbf{E}\mathbf{S} + \mathbf{S}\mathbf{E}$. We must account for permutations (relabeling)

▶ Set of **relative error matrices** modulo permutation. Matrices $\tilde{\mathbf{E}}$ are symmetric, $\tilde{\mathbf{E}} = \tilde{\mathbf{E}}^T$

$$\mathcal{E}(\mathbf{S}, \hat{\mathbf{S}}) = \left\{ \tilde{\mathbf{E}} : \mathbf{P}^T \hat{\mathbf{S}} \mathbf{P} = \mathbf{S} + \tilde{\mathbf{E}}\mathbf{S} + \mathbf{S}\tilde{\mathbf{E}}, \mathbf{P} \in \mathcal{P} \right\}$$

▶ **Relative error matrix modulo permutation** is the one with smallest norm $\Rightarrow \mathbf{E} = \underset{\tilde{\mathbf{E}} \in \mathcal{E}(\mathbf{S}, \hat{\mathbf{S}})}{\operatorname{argmin}} \|\tilde{\mathbf{E}}\|$

▶ Define **relative distance modulo permutation** as $\Rightarrow d(\mathbf{S}, \hat{\mathbf{S}}) = \|\mathbf{E}\| = \min_{\tilde{\mathbf{E}} \in \mathcal{E}(\mathbf{S}, \hat{\mathbf{S}})} \|\tilde{\mathbf{E}}\|$

▶ Norm $\|\mathbf{E}\| = d(\mathbf{S}, \hat{\mathbf{S}})$ is a **relative measure** of how far $\hat{\mathbf{S}}$ is from **being a permutation** of \mathbf{S}

- ▶ Relative perturbations tie **changes in the edge weights** to the **local structure** of the graph
- ▶ Compare edge weights in the given matrix **S** and the permuted version of the perturbations **\hat{S}**

$$\begin{aligned} \left(\mathbf{P}^T \hat{\mathbf{S}} \mathbf{P} \right)_{ij} &= S_{ij} + \left(\mathbf{E} \mathbf{S} \right)_{ij} + \left(\mathbf{S} \mathbf{E} \right)_{ij} \\ &= S_{ij} + \sum_{k \in n(j)} E_{ik} S_{kj} + \sum_{k \in n(i)} S_{ik} E_{kj} \end{aligned}$$

- ▶ Edge changes are proportional to the **degree of the incident nodes**. Scaled by entries of error matrix
- ▶ Parts of the graph with **weaker connectivity** see **smaller changes** than parts with **stronger links**
- ▶ In **generic additive perturbations** weights can change the same **regardless of local connectivity**

Stability of Integral Lipschitz Filters to Relative Perturbations

- ▶ We show that integral Lipschitz filters are stable to relative perturbations of the graph support.

Theorem (Integral Lipschitz Filters are Stable to Relative Perturbations)

Consider **graph filter \mathbf{h}** along with shift operators **\mathbf{S}** and **$\hat{\mathbf{S}}$** having **n nodes**. If it holds that:

(H1) **\mathbf{S}** and **$\hat{\mathbf{S}}$** are related by **$\mathbf{P}^T \hat{\mathbf{S}} \mathbf{P} = \mathbf{S} + \mathbf{E} \mathbf{S} + \mathbf{S} \mathbf{E}$** with **$\mathbf{P}$** a permutation matrix

(H2) **Error matrix** has norm **$\|\mathbf{E}\| = \epsilon$** and **eigenvector misalignment constant δ** relative to **\mathbf{S}**

(H3) The filter is **integral Lipschitz** with constant **C**

Then, the operator distance modulo permutation between filters **$\mathbf{H}(\mathbf{S})$** and **$\mathbf{H}(\hat{\mathbf{S}})$** is bounded by

$$\|\mathbf{H}(\hat{\mathbf{S}}) - \mathbf{H}(\mathbf{S})\|_{\mathcal{P}} \leq 2C (1 + \delta\sqrt{n}) \epsilon + \mathcal{O}(\epsilon^2).$$

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- ▶ Save for the 2 factor, it is the **same bound** we have for the case of **additive perturbations**.
- ▶ The difference is in **hypotheses (H1) and (H3)**. Hypothesis (H2) does not change
 - (H1)** The **perturbation is relative**. $\Rightarrow \mathbf{P}^T \hat{\mathbf{S}} \mathbf{P} = \mathbf{S} + \mathbf{E} \mathbf{S} + \mathbf{S} \mathbf{E}$. **Not additive**.
 - (H3)** The filter is **integral Lipschitz** with constant C . **Not regular Lipschitz**.

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$$\|\mathbf{H}(\hat{\mathbf{S}}) - \mathbf{H}(\mathbf{S})\|_{\mathcal{P}} \leq 2C (1 + \delta\sqrt{n}) \epsilon + \mathcal{O}(\epsilon^2).$$

- ▶ If \mathbf{S} and $\hat{\mathbf{S}}$ are ϵ -close in relative terms, the filters $\mathbf{H}(\mathbf{S})$ and $\mathbf{H}(\hat{\mathbf{S}})$ are ϵ -close. Modulo permutation
- ▶ Proportional to the integral Lipschitz constant of the filter's frequency response.
- ▶ Proportional to $(1 + \delta\sqrt{n})$. Not great for large graphs. Unless the misalignment decreases with n .

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- ▶ Filter perturbations are first order **Lipschitz continuous** with respect to the **perturbation's size ϵ**
⇒ With **Lipschitz** constant ⇒ $2C (1 + \delta\sqrt{n})$
- ▶ Stronger than plain continuity. Which would say “output changes are small if input changes are”
- ▶ Input perturbation measure is **relative** ⇒ Norm $\|\mathbf{E}\| = \epsilon$ in **multiplicative** perturbation $\mathbf{E}\mathbf{S} + \mathbf{S}\mathbf{E}$

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$$\|\mathbf{H}(\hat{\mathbf{S}}) - \mathbf{H}(\mathbf{S})\|_{\mathcal{P}} \leq 2C (1 + \delta\sqrt{n}) \epsilon + \mathcal{O}(\epsilon^2).$$

- ▶ Bound is universal for all graphs with a given number of nodes n . Bound depends on:
 - ⇒ A property of the filter's frequency response. The filter's integral Lipschitz constant C
 - ⇒ And properties of the perturbation \mathbf{E} . The eigenvector misalignment δ and the norm $\|\mathbf{E}\| = \epsilon$
- ▶ There is no constant in the bound that depends on the graph shift operator \mathbf{S} . Save for n .

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The operator distance modulo permutation between filters $\mathbf{H}(\mathbf{S})$ and $\mathbf{H}(\hat{\mathbf{S}})$ is bounded by

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- ▶ Eigenvector misalignment δ is a property of the perturbation matrix. Independent of filter choice
- ▶ Meaningless asymptotically on n . Growth is not terrible. It is at most $1 + 8\sqrt{n}$

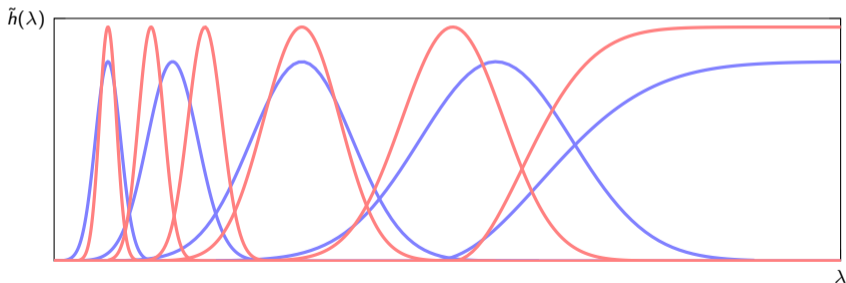
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- ▶ Bound depends on **integral Lipschitz constant C** . Very different from Lipschitz constant
- ▶ Can decrease C to increase stability. But effect on **Discriminability** depends on the **frequency**.
 - ⇒ Discriminative at low frequencies regardless of C
 - ⇒ Non-discriminative at high frequencies regardless of C

- ▶ Stability to **relative perturbations** requires **integral Lipschitz filters**. As in the case of dilations
- ▶ No stability vs discriminability tradeoff \Rightarrow Stability and discriminability are incompatible
- ▶ **No discriminability for large λ** . Regardless of how much instability we tolerate by increasing C .



Stability Properties of Graph Neural Networks

- ▶ The stability properties we studied for graph filters are inherited by GNNs

- ▶ We proved that integral Lipschitz filters are stable to dilations of the shift operator

Theorem (Integral Lipschitz Graph Filters are Stable to Scaling)

Given graph shift operators \mathbf{S} and $\hat{\mathbf{S}} = (1 + \epsilon)\mathbf{S}$ and an **integral Lipschitz** filter with constant C .

The operator norm difference between filters $\mathbf{H}(\mathbf{S})$ and $\mathbf{H}(\hat{\mathbf{S}})$ is bounded as

$$\|\mathbf{H}(\hat{\mathbf{S}}) - \mathbf{H}(\mathbf{S})\| \leq C\epsilon + \mathcal{O}(\epsilon^2).$$

- ▶ And that GNNs with integral Lipschitz layers **inherit** the stability of the filters to these dilations

Theorem (Integral Lipschitz GNNs are Stable to Scaling)

Given shift operators \mathbf{S} and $\hat{\mathbf{S}} = (1 + \epsilon)\mathbf{S}$ and a GNN operator $\Phi(\cdot; \mathbf{S}, \mathcal{H})$ with L **single-feature layers**. The filters at each layer have unit operator norms and are **integral Lipschitz** with constant C . The nonlinearity σ is normalized Lipschitz. Then

$$\| \Phi(\cdot; \hat{\mathbf{S}}, \mathcal{H}) - \Phi(\cdot; \mathbf{S}, \mathcal{H}) \| \leq C L \epsilon + \mathcal{O}(\epsilon^2).$$

- ▶ The proof has **nothing that is specific to dilations**
 - ⇒ **Any** stability property that a **class** of graph filters has is **inherited** to a respective GNN

Theorem (Integral Lipschitz GNNs are Stable to Scaling)

Given shift operators \mathbf{S} and $\hat{\mathbf{S}} = (1 + \epsilon)\mathbf{S}$ and a GNN operator $\Phi(\cdot; \mathbf{S}, \mathcal{H})$ with L single-feature layers. **The filters at each layer** have unit operator norms and **are integral Lipschitz with constant C** . The nonlinearity σ is normalized Lipschitz. Then

$$\|\Phi(\cdot; \hat{\mathbf{S}}, \mathcal{H}) - \Phi(\cdot; \mathbf{S}, \mathcal{H})\| \leq C L \epsilon + O(\epsilon^2).$$

- ▶ **Lipschitz filters** are stable to **additive** deformations of the shift operator
 - ⇒ **GNNs with Lipschitz layers** are stable to **additive** deformations of the shift operator

- ▶ **Integral Lipschitz filters** are stable to **relative** deformations of the shift operator
 - ⇒ **GNNs with integral Lipschitz layers** are stable to **relative** deformations of the shift operator

- ▶ Reminders and precision are redundant but not unnecessary. **Normalize** filters and nonlinearities.
- ▶ At each layer of the GNN, the **filters have unit operator norm** $\Rightarrow \|\mathbf{H}_\ell(\mathbf{S})\| = 1$
 - \Rightarrow Easy to achieve with scaling \Rightarrow Equivalent to $\max_{\lambda} \tilde{h}_\ell(\lambda) = 1$
- ▶ The **nonlinearity** σ is Lipschitz and **normalized** so that $\Rightarrow \|\sigma(\mathbf{x}_2) - \sigma(\mathbf{x}_1)\| \leq \|\mathbf{x}_2 - \mathbf{x}_1\|$
 - \Rightarrow Easy to achieve with scaling. True of ReLU, hyperbolic tangent, and absolute value
- ▶ Joining both assumptions \Rightarrow If **input energy is** $\|\mathbf{x}\| \leq 1$, all layer outputs have energy $\|\mathbf{x}_\ell\| \leq 1$

Theorem (GNN Stability to Additive Perturbations)

Consider a GNN operator $\Phi(\cdot; \mathbf{S}, \mathcal{H})$ along with shifts operators \mathbf{S} and $\hat{\mathbf{S}}$ having n nodes. If:

- (H1) Shift operators are related by $\mathbf{P}^T \hat{\mathbf{S}} \mathbf{P} = \mathbf{S} + \mathbf{E}$. With \mathbf{P} a permutation matrix
- (H2) The error matrix \mathbf{E} has norm $\|\mathbf{E}\| = \epsilon$ and eigenvector misalignment δ relative to \mathbf{S}
- (H3) The GNN has L single-feature layers with Lipschitz filters with constant C
- (H4) Filters have unit operator norm and the nonlinearity is normalized Lipschitz

Then, the operator distance modulo permutation between $\Phi(\cdot; \mathbf{S}, \mathcal{H})$ and $\Phi(\cdot; \hat{\mathbf{S}}, \mathcal{H})$ is bounded by

$$\|\Phi(\cdot; \hat{\mathbf{S}}, \mathcal{H}) - \Phi(\cdot; \mathbf{S}, \mathcal{H})\|_{\mathcal{P}} \leq C (1 + \delta\sqrt{n}) L\epsilon + \mathcal{O}(\epsilon^2).$$

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- ▶ It is **essentially the same bound** we have for the case of Lipschitz filters. **Propagated over L layers**
- ▶ A GNN in which layers are made up of Lipschitz **inherits** the stability of the Lipschitz filter class
- ▶ The nonlinearity is **pointwise** \Rightarrow Graph deformations have **no effect** on its action

Theorem (GNN Stability to Relative Perturbations)

Consider a GNN operator $\Phi(\cdot; \mathbf{S}, \mathcal{H})$ along with shifts operators \mathbf{S} and $\hat{\mathbf{S}}$ having n nodes. If:

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(H2) The error matrix \mathbf{E} has norm $\|\mathbf{E}\| = \epsilon$ and eigenvector misalignment δ relative to \mathbf{S}

(H3) The GNN has L single-feature layers with integral Lipschitz filters with constant C

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Then, the operator distance modulo permutation between $\Phi(\cdot; \mathbf{S}, \mathcal{H})$ and $\Phi(\cdot; \hat{\mathbf{S}}, \mathcal{H})$ is bounded by

$$\|\Phi(\cdot; \hat{\mathbf{S}}, \mathcal{H}) - \Phi(\cdot; \mathbf{S}, \mathcal{H})\|_{\mathcal{P}} \leq 2C (1 + \delta\sqrt{n}) L\epsilon + \mathcal{O}(\epsilon^2).$$

Theorem (Single Feature GNN Stability to Relative Perturbations)

The operator distance modulo permutation between $\Phi(\cdot; \mathbf{S}, \mathcal{H})$ and $\Phi(\cdot; \hat{\mathbf{S}}, \mathcal{H})$ is bounded by

$$\|\Phi(\cdot; \hat{\mathbf{S}}, \mathbf{h}) - \Phi(\cdot; \mathbf{S}, \mathbf{h})\|_{\mathcal{P}} \leq 2C (1 + \delta\sqrt{n}) L\epsilon + \mathcal{O}(\epsilon^2).$$

- ▶ It is **essentially the same bound** we have for integral Lipschitz filters. **Propagated over L layers**
- ▶ A GNN in which layers are integral Lipschitz **inherits** the stability of integral Lipschitz filters
- ▶ The nonlinearity is **pointwise** \Rightarrow Graph deformations have **no effect** on its action

GNNs Inherit the Stability Properties of Graph Filters

- ▶ Let's do the proof for relative perturbations and integral Lipschitz filters.
- ▶ But this time we pay attention to the fact that steps apply to any stability claim on any filter class.
- ▶ And take the chance to discuss how GNNs inherit their stability properties from graph filters

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Consider a GNN operator $\Phi(\cdot; \mathbf{S}, \mathcal{H})$ along with shifts operators \mathbf{S} and $\hat{\mathbf{S}}$ having n nodes. If:

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Then, the operator distance modulo permutation between $\Phi(\cdot; \mathbf{S}, \mathcal{H})$ and $\Phi(\cdot; \hat{\mathbf{S}}, \mathcal{H})$ is bounded by

$$\|\Phi(\cdot; \hat{\mathbf{S}}, \mathcal{H}) - \Phi(\cdot; \mathbf{S}, \mathcal{H})\|_{\mathcal{P}} \leq 2C (1 + \delta\sqrt{n}) L\epsilon + \mathcal{O}(\epsilon^2).$$

Proof: Let \mathbf{x}_ℓ be the Layer ℓ output of GNN $\Phi(\mathbf{x}; \mathbf{S}, \mathcal{H})$. Input signal \mathbf{x} with $\|\mathbf{x}\| = 1$

Let $\hat{\mathbf{x}}_\ell$ be the Layer ℓ output of GNN $\Phi(\mathbf{x}; \hat{\mathbf{S}}, \mathcal{H})$. Input signal \mathbf{x} with $\|\mathbf{x}\| = 1$

- ▶ Layer ℓ is a perceptron with filter $\mathbf{H}_\ell \Rightarrow \|\hat{\mathbf{x}}_\ell - \mathbf{x}_\ell\| = \left\| \sigma \left[\mathbf{H}_\ell(\hat{\mathbf{S}})\hat{\mathbf{x}}_{\ell-1} \right] - \sigma \left[\mathbf{H}_\ell(\mathbf{S})\mathbf{x}_{\ell-1} \right] \right\|$
- ▶ Nonlinearity is **normalized Lipschitz** $\Rightarrow \|\hat{\mathbf{x}}_\ell - \mathbf{x}_\ell\| \leq \left\| \mathbf{H}_\ell(\hat{\mathbf{S}})\hat{\mathbf{x}}_{\ell-1} - \mathbf{H}_\ell(\mathbf{S})\mathbf{x}_{\ell-1} \right\|$
- ▶ This is the **critical step** of the proof. The rest of the proof is just algebra.

- ▶ In last bound, add and subtract $\mathbf{H}_\ell(\hat{\mathbf{S}})\mathbf{x}_{\ell-1}$. Triangle inequality. Submultiplicative property of norms

$$\begin{aligned} \|\hat{\mathbf{x}}_\ell - \mathbf{x}_\ell\| &\leq \left\| \mathbf{H}_\ell(\hat{\mathbf{S}})\hat{\mathbf{x}}_{\ell-1} - \mathbf{H}_\ell(\mathbf{S})\mathbf{x}_{\ell-1} + \mathbf{H}_\ell(\hat{\mathbf{S}})\mathbf{x}_{\ell-1} - \mathbf{H}_\ell(\hat{\mathbf{S}})\mathbf{x}_{\ell-1} \right\| \\ &\leq \left\| \mathbf{H}_\ell(\hat{\mathbf{S}}) - \mathbf{H}_\ell(\mathbf{S}) \right\| \times \left\| \mathbf{x}_{\ell-1} \right\| + \left\| \mathbf{H}_\ell(\hat{\mathbf{S}}) \right\| \times \left\| \hat{\mathbf{x}}_{\ell-1} - \mathbf{x}_{\ell-1} \right\| \end{aligned}$$

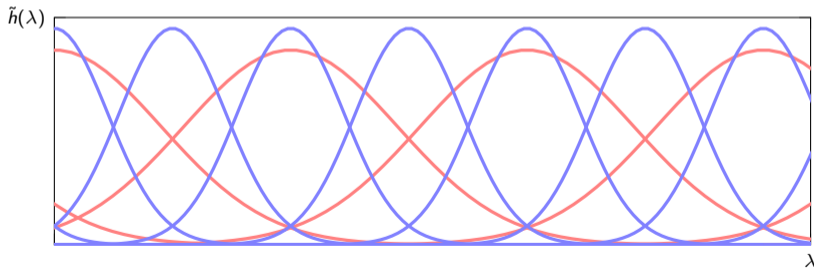
- ▶ Since **filters are normalized** \Rightarrow Filter norm $\|\mathbf{H}_\ell(\hat{\mathbf{S}})\| = 1$. Signal norm $\Rightarrow \|\mathbf{x}_{\ell-1}\| \leq 1$
- ▶ **Relative perturbations and integral Lipschitz** $\Rightarrow \|\mathbf{H}_\ell(\hat{\mathbf{S}}) - \mathbf{H}_\ell(\mathbf{S})\| \leq 2C(1 + \delta\sqrt{n})\epsilon + \mathcal{O}(\epsilon^2)$
- ▶ Put all bounds together $\Rightarrow \|\hat{\mathbf{x}}_\ell - \mathbf{x}_\ell\| \leq 2C(1 + \delta\sqrt{n})\epsilon \times 1 + 1 \times \|\hat{\mathbf{x}}_{\ell-1} - \mathbf{x}_{\ell-1}\| + \mathcal{O}(\epsilon^2)$
- ▶ Apply **recursively** from Layer L back to Layer 1. The L factor appears ■

GNNs Inherit the Stability of Graph Filters

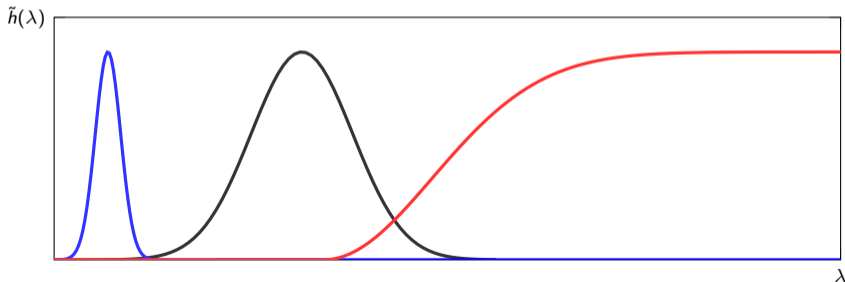
Since Stability is **inherited** from graph filters, **mutatis mutandis**, the same observations hold here.

- ▶ We claim **stability**. Which is stronger than continuity.
- ▶ The stability bounds are **universal** for all graphs with a given number of nodes
- ▶ Bounds depend on **filter's Lipschitz constant C** and the **number of layers L** . Which we control.
- ▶ And the eigenvector misalignment constant. Which we don't control. Depends on the perturbation.

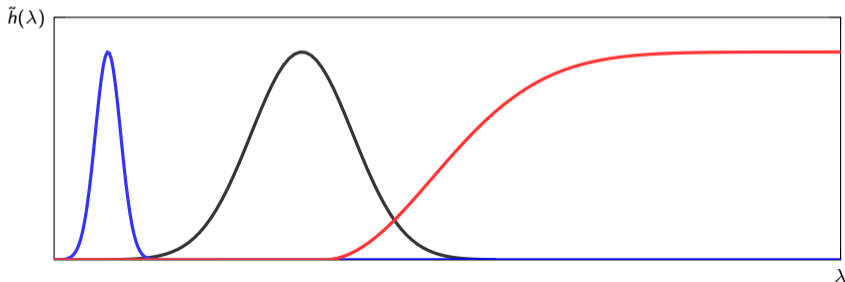
- ▶ GNNs whose layers are made up of Lipschitz graph filters are stable to additive deformations
- ▶ This is good news \Rightarrow We have a genuine stability vs discriminability tradeoff
- ▶ Alas, **a bit of a mirage** \Rightarrow Graph perturbations are more naturally measured in relative terms



- ▶ **Meaningful** stability claims with respect to **relative** perturbations require **integral Lipschitz** filters.
- ▶ Integral Lipschitz filters **have to be flat at high frequencies**. \Rightarrow They **can't discriminate**
- ▶ It is **impossible to separate** signals with high frequency features **and be stable** to deformations



- ▶ **Meaningful** stability claims with respect to **relative** perturbations require **integral Lipschitz** filters.
- ▶ On the flip side, integral Lipschitz filter can be **very sharp at low frequencies**
- ▶ We can be **very discriminative** at low frequencies. And at the same **very stable** to deformations



- ▶ GNNs use **low-pass nonlinearities** to demodulate **high frequencies** into **low frequencies**
- ▶ Where they can be **discriminated sharply with a stable filter** at the next layer
- ▶ Thus, they **can be stable and discriminative**. Something that **linear graph filters can't be**

