Graphons

- We introduce graphons to study graph filters and GNNs in the limit of large number of nodes

Definition (Graphon)

A graphon is a bounded symmetric measurable function $\Rightarrow \mathrm{W} : [0, 1]^2 \rightarrow [0, 1]$

- Can think of a graphon as a weighted symmetric graph with uncountable nodes

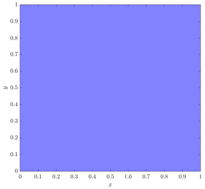
$\Rightarrow$ The labels are the graphon arguments $\Rightarrow u \in [0, 1]$.

$\Rightarrow$ The weights are the graphon values $\Rightarrow W(u, v) = W(v, u)$

Graphon Examples

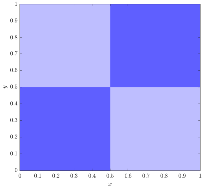
> **Definition (Graphon)**
>
> A graphon is a bounded symmetric measurable function $\Rightarrow W : [0,1]^2 \rightarrow [0,1]$

Uniform (Erdős-Rényi)



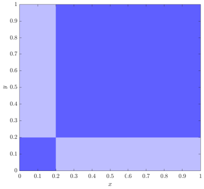
$W(u,v) = p$

Balanced stochastic block model (SBM)



$W(u,v) = p \gg W(u,v) = q$

Unbalanced (SBM)



$W(u,v) = p \gg W(u,v) = q$

The Purpose of a Graphon

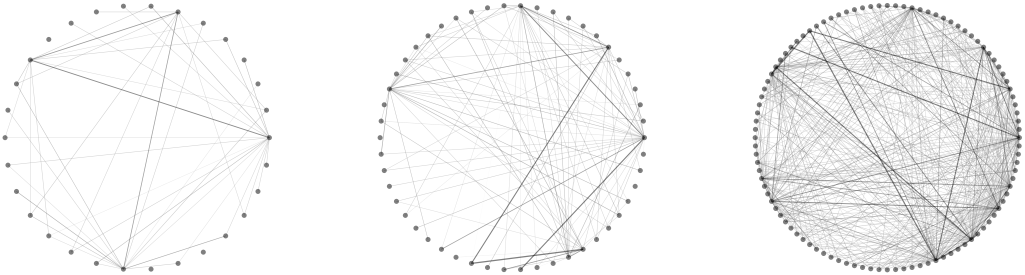
Definition (Graphon)

A graphon is a bounded symmetric measurable function $\Rightarrow W : [0,1]^2 \to [0,1]$

- Practice $\Rightarrow$ Graph sets where graphs in the set have large number of nodes and similar structure
- Theory $\Rightarrow$ A generative model of graph families via deterministic or stochastic edge sampling
- Theory $\Rightarrow$ A limit object for a sequence of graphs

The Product Similarity "Graphon"

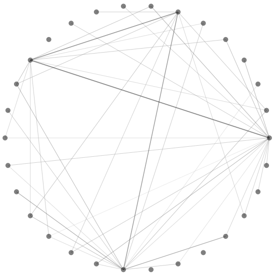
- Product similarity graphs, even with different number of nodes, "look like each other"
- Abstract similarities between graphs into a limit object $\Rightarrow$ The product similarity "graphon"



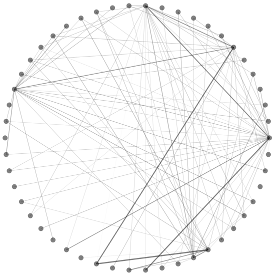
$n = 30$ products　　$n = 50$ products　　$n = 100$ products

- We never compute the product similarity "graphon"

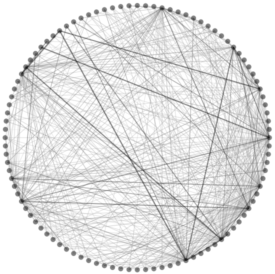
  $\Rightarrow$ Use abstract idea of graphon to work with all of these graphs as if they were the same object



$n = 30$ products



$n = 50$ products



$n = 100$ products

- Vertices: For an n-node graph, sample n points $\{u_1, u_2, \ldots, u_n\}$ from the unit interval $[0, 1]$

  $\Rightarrow$ Points can be sampled on a grid, uniformly at random, etc.

  $\Rightarrow$ Each sample u_i corresponds to a node $i \in \{1, 2, 3, \ldots, n\}$ of the graph

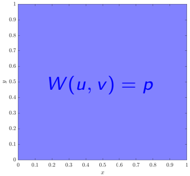
- Edges: Evaluate $\mathrm{W}(u_i, u_j)$ for edge (i, j)

  $\Rightarrow$ Stochastic: Connect i and j with an unweighted undirected edge with probability $\mathrm{W}(u_i, u_j)$

  $\Rightarrow$ Weighted: Connect i and j with weighted undirected edge with weight $\mathrm{W}(u_i, u_j)$

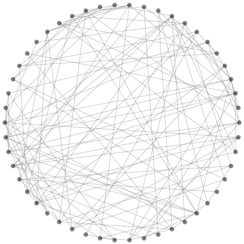
Uniform Graphons as Generative Models

- Use uniform Graphon



To generate random graphs with the same

Or different number of nodes



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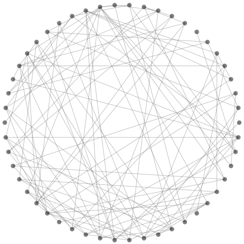

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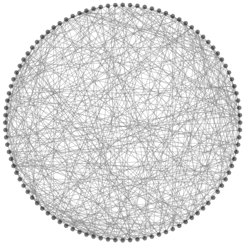
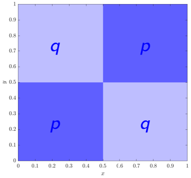


$n = 100$ nodes

Balanced SBM Graphons as Generative Models

- Use balanced SBM

Graphon



To generate balanced SBM graphs with the same

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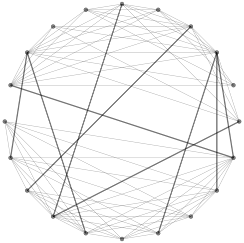
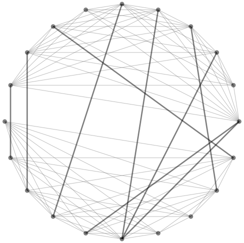


$n = 20$ nodes



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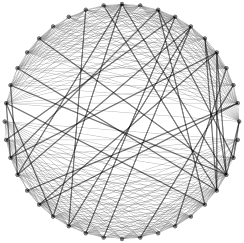
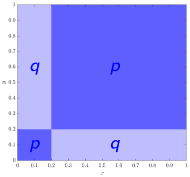


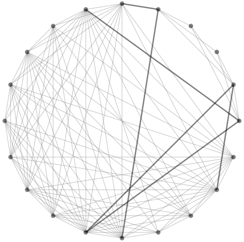
$n = 40$ nodes

Unbalanced SBM Graphons as Generative Models

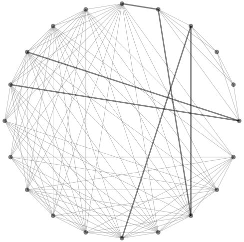
- Use Unbalanced SBM Graphon



To generate unbalanced SBM graphs with the same Or different number of nodes



$n = 20$ nodes



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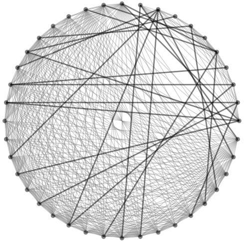
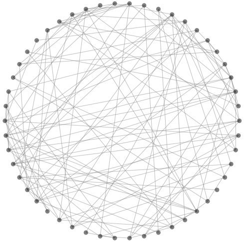


$n = 40$ nodes

- As we consider random graphs with larger numbers of nodes the graphs approach a limit

$\Rightarrow$ It is unclear what that limit is. The graphon is the limit. As we will see



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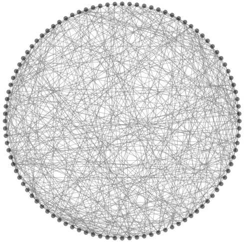

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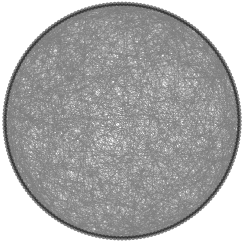
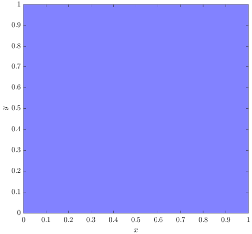


$n = 200$ nodes $\rightarrow$



Graphon $W(u, v) = p$

Convergence of Graph Sequences

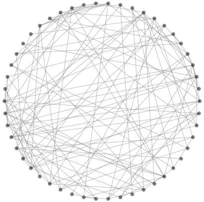
- A graphon is the limit of a sequence of graphs that converges in terms of homomorphism densities

Convergent Graph Sequences

- Sequence of graphs with growing number of nodes n $\Rightarrow \left\{ G_n = (V_n, E_n, S_n) \right\}_{n=1}^{\infty}$.

- The graph sequence $\{G_n\}_{n=1}^{\infty}$ converges to a graphon W $\Rightarrow$ In what sense?

  $\Rightarrow$ We need to introduce three concepts: Motifs, homomorphisms, and homomorphism densities



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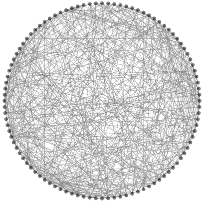

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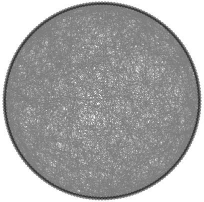

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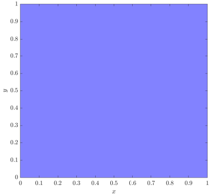
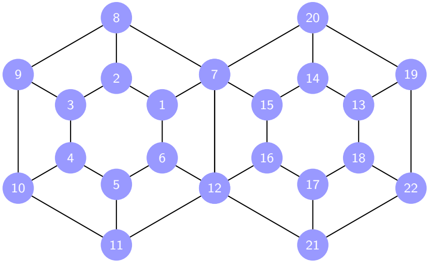


Graphon $W(u, v) = p$

- A motif F is a graph. But think of it as a small graph that we embed in another larger graph



- Homomorphisms are adjacency preserving maps from motif $F = (V', E')$ into graph $G = (V, E)$

$$\beta : V' \rightarrow V \text{ such that } \Big(i, j\Big) \in E' \text{ implies } \Big(\beta(i), \beta(j)\Big) \in E$$

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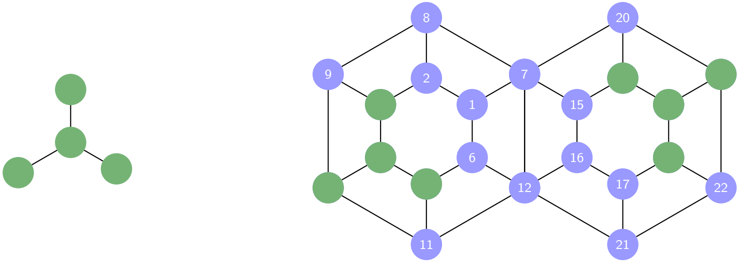

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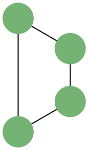

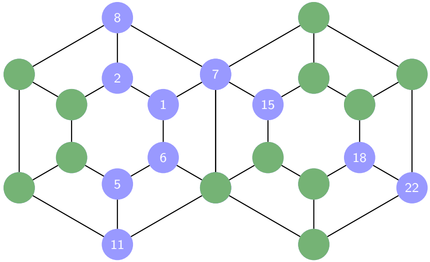

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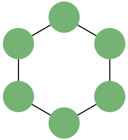

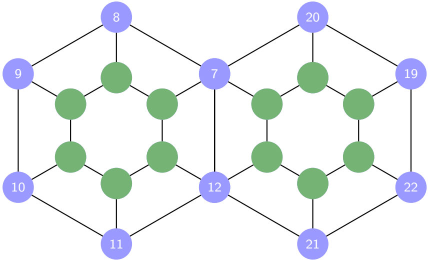

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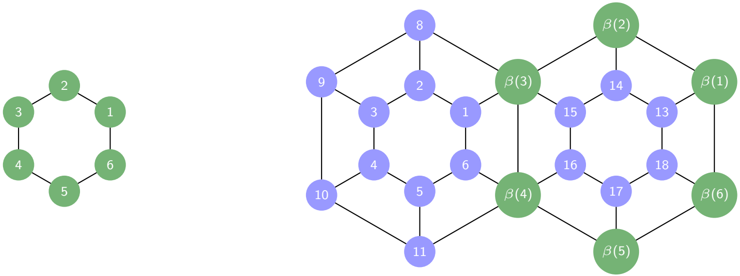

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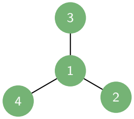
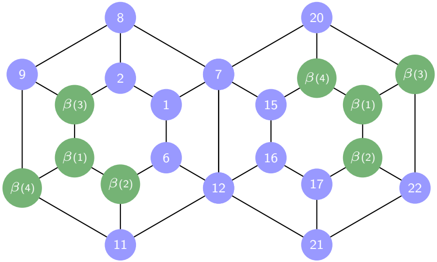
- Given motif F and graph G, there are multiple homomorphism functions β





- We define $\text{hom}(F, G)$ to represent the number of homomorphisms between motif F and graph G

- If the graph G has n nodes and the motif F has n' nodes, there are $n^{n'}$ different maps from F to G

- Homomorphism density of motif F in graph G is the fraction of maps that are homomorphisms

$$t(F, G) = \frac{\text{hom}(F, G)}{n^{n'}}$$

- Density $t(F, G)$ is a relative measure of the number of ways in in which F can be mapped into G

Homomorphism Density for Weighted Graphs

- Consider weighted graph $G = (V, E, S)$ with adjacency matrix S

- Homomorphism density of motif F in weighted graph G with the adjacency matrix S is

$$t(F, G) \; = \; = \frac{\sum_{\beta} \prod_{(i,j)\in\mathcal{E}'} [\mathsf{S}]_{\beta(i)\beta(j)}}{n^{n'}}$$

- Weight each motif embedding by the product of the edge weights in the homomorphism image.

- The Homomorphism density of a motif F into a given graphon W is defined as

$$t(F, W) = \int_{[0,1]^{n'}} \prod_{(i,j)\in\mathcal{E}'} W(u_i, u_j) \prod_{i\in\mathcal{V}'} du_i$$

- The homomorphism density is the probability of drawing the motif F from the graphon W

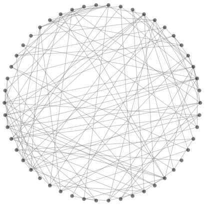
Definition (Convergent graph sequence)

A sequence of undirected graphs G_n converges to the graphon W if and only if for all motifs F

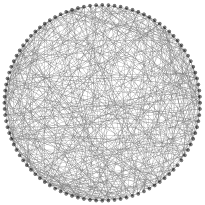
$$\lim_{n \to \infty} t(F, G_n) = t(F, W)$$

- We say that the sequence G_n converges to W in the homomorphism density sense
- It can be proven that every graphon is the limit object of a sequence of convergent graphs
- It can be proven that every convergent graph sequence converges to a graphon

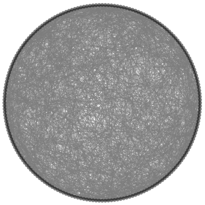
- Consider a sequence of random graphs $\{G_n\}$ sampled from the graphon W. Graphs G_n have
  - $\Rightarrow$ Labels $u_i \sim U[0,1]$ drawn uniformly at random from the interval $[0,1]$
  - $\Rightarrow$ Edge sets such that $(u_i, u_j) \in \mathcal{E}$ with probability $W(u_i, u_j)$
- We have $\lim_{n\to\infty} t(F, G_n) = t(F, W)$ in the homomorphism density sense almost surely



$n = 50$ nodes $\rightarrow$



$n = 100$ nodes $\rightarrow$



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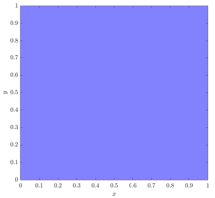
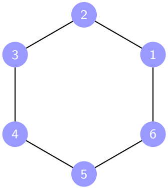


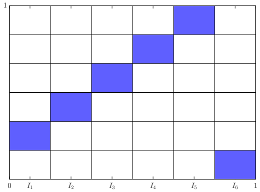
Graphon $W(u,v) = p$

- Every undirected graph admits a graphon representation which we call its induced graphon
- Consider a graph $G = \{\mathcal{V}, \mathcal{E}, \mathbf{S}\}$ with $|\mathcal{V}| = n$ and normalized graph shift operator $\mathbf{S}$
- Regular partition of the unit interval with n subintervals $\Rightarrow \mathrm{I}_i = \Big[(i-1)/n,\ i/n\Big)$
- We define the induced graphon $W_G \Rightarrow W_G(u,v) = [\mathbf{S}]_{ij}\ \mathbb{I}(u \in \mathrm{I}_i)\ \mathbb{I}(v \in \mathrm{I}_j)$



Cycle graph G with $n = 6$ nodes

$\rightarrow$

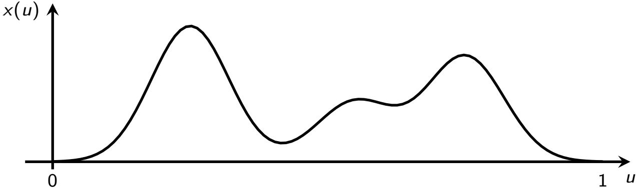


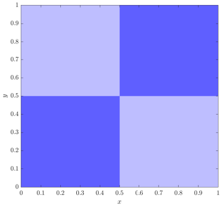
Graphon W_G induced by the graph G

Graphon Signals

- Graph signals are signals supported on graphons. They are limit objects of graph signals

- Graphon signals are pairs (W, X) where W is a graphon and $X : [0,1] \to \mathbb{R}$ is a function
- Function $X(u) \in L^2([0,1])$ has finite energy $\Rightarrow \int_0^1 |X(u)|^2 du < \infty$.



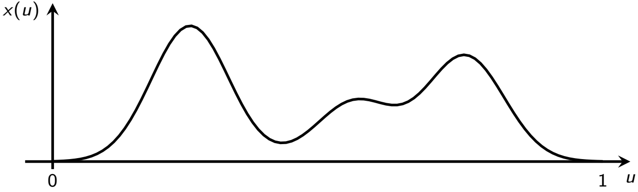


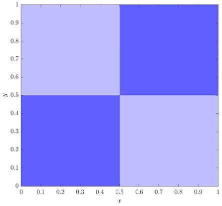
- Generative models of graph signals. And limits of convergent sequences of graph signals

- We generate graph signals $(\mathbf{S}_n, \mathbf{x}_n)$ by taking n samples of the graphon signal (W, X)

- Sample the graphon at node labels u_i. Sample the function X at node labels u_i $\Rightarrow x_i = X(u_i)$

- Graph signal sampled from the unit interval in the same coordinates u_i where graphon is sampled





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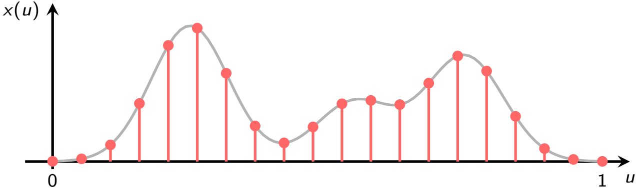
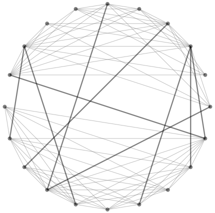
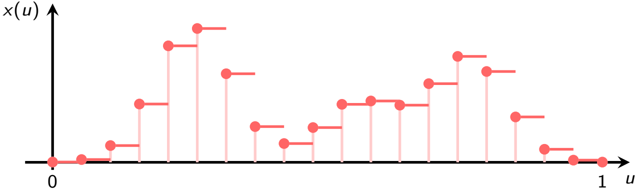


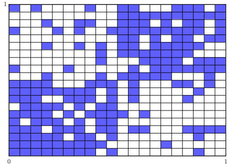


- Every graph signal x supported on graph G induces a graphon signal (W_G, X_G)
- Regular partition of unit interval with n subintervals $\mathrm{I}_i = \left[(i-1)/n,\ i/n\right)$

$\Rightarrow$ Induced signal $X_G(u) = x_i\, \mathbb{I}(u \in I_i)$

$\Rightarrow$ W_G is the graphon induced by the graph G $\Rightarrow$ $W_G(u,v) = [\mathbf{S}]_{ij}\ \mathbb{I}(u \in \mathrm{I}_i)\ \mathbb{I}(v \in \mathrm{I}_j)$





Definition (Convergent sequences of graph signals)

A sequence of graph signals $(G_n, \mathbf{x}_n)$ is said to converge to the graphon signal (W, X), if there exists a sequence of permutations π_n such that for all motifs F we have

$$t(F, G_n) \to t(F, W), \qquad \text{and} \left\| X_{\pi_n(G_n)} - X \right\|_{L^2} \to 0$$

We say (W, X) is the limit of the graph signal sequence and write $(G_n, x_n) \to (W, X)$

- The permutation is used here to make the convergence definition independent of labels
- To enable comparison of the vector $\mathbf{x}_n$ and the function X we use the induced signal in the L_2 norm

- The Graphon W can be used to define an integral linear operator $\Rightarrow T_W : L^2([0,1]) \to L^2([0,1])$

- When applied to the graphon signal X, the operator T_W produces the signal $T_W X$ with values

$$(T_W X)(v) = \int_0^1 W(u,v)X(u)\, du$$

- This is a Hilbert-Schmidt operator because W is bounded and compact. It's a matrix multiplication

- We say that the linear operator T_W is the graphon shift operator (WSO) of the graphon W

$\Rightarrow$ Applying the WSO T_W to the graphon signal X diffuses X over the graphon W

Graphon Fourier Transform

- We define a graphon Fourier transform to enable spectral representation of graphon signals.

- The WSO is a self adjoint Hilbert-Schmidt operator $\Rightarrow (T_{\mathrm{W}}X)(v) = \int_0^1 \mathrm{W}(u, v)X(u)\, du$

- The function $\varphi : [0, 1] \to \mathbb{R}$ is an eigenfunction of T_W with associated eigenvalue λ if

$$(T_{\mathrm{W}}\varphi)(v) \;=\; \int_0^1 \mathrm{W}(u, v)\varphi(u)\, du \;=\; \lambda\varphi(v)$$

- T_{W} has a countable number of eigenvalue-eigenfunction pairs $\Rightarrow \Big\{ (\lambda_i, \varphi_i) \Big\}_{i=1}^{\infty}$

- We assume eigenfunctions are normalized to unit energy $\Rightarrow \|\varphi_i\|^2 = \int_0^1 \varphi(u)du = 1$

- The (countable number of) eigenfunctions of the operator T_w are an orthonormal basis of $L^2([0,1])$

- We can thus decompose the graphon W in the basis $\{\varphi_i\}_{i=1}^{\infty}$ of eigenfunctions of the operator T_W

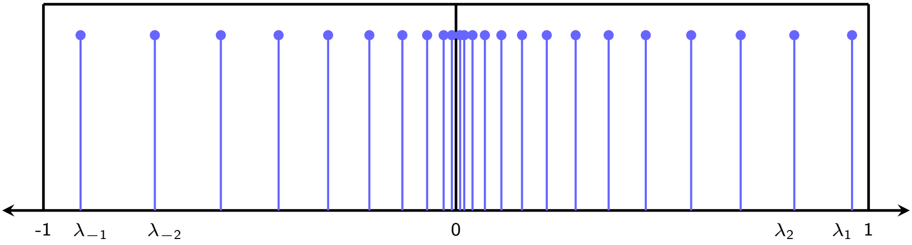
$$\mathrm{W}(u,v) \;=\; \sum_{i=0}^{\infty} \lambda_i \, \varphi_i(u) \, \varphi_i(v)$$

- More or less the same as the eigenvector decomposition $\Rightarrow \mathrm{S} \;=\; \mathrm{V}\Lambda\mathrm{V}^H \;=\; \sum_{i=0}^{\infty} \lambda_i \, \mathrm{v}_i \, \mathrm{v}_i^T$

The Range of the Graphon Eigenvalues

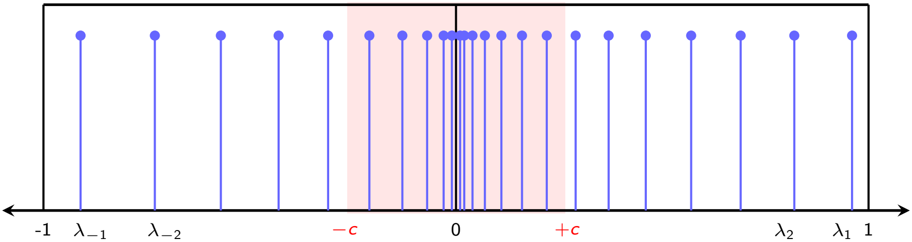
- T_W is self adjoint and $0 \leq W(x,y) \leq 1$ $\Rightarrow$ Eigenvalues are real and lie in the interval $[-1, 1]$

- Order them as $\Rightarrow -1 \leq \lambda_{-1} \leq \lambda_{-2} \leq \ldots \leq 0 \leq \ldots \leq \lambda_2 \leq \lambda_1 \leq 1$



Eigenvalues Concentrate Around Zero

- Graphon eigenvalues accumulate at $\lambda = 0$ $\Rightarrow \lim_{i\to\infty} \lambda_i = \lim_{i\to\infty} \lambda_{-i} = 0$. And only at $\lambda = 0$
- For any $c > 0$, the number of eigenvalues with $|\lambda_i| \geq c$ is finite $\Rightarrow \#\left\{\lambda_i : |\lambda_i| \geq c\right\} = n_c < \infty$
- All eigenvalues that are not $\lambda_j = 0$ have finite multiplicity



Theorem (Eigenvalue Convergence of a Graph Sequence)

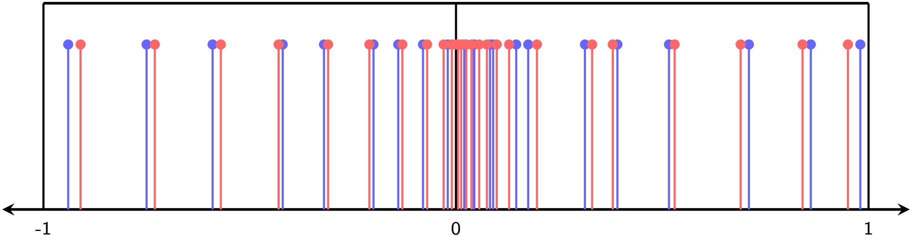
If a graph sequence $\{G_n\}$ converges to a graphon W in the homomorphism density sense , then

$$\lim_{n\to\infty} \frac{\lambda_j(S_n)}{n} = \lambda_j(T_W) = \lim_{n\to\infty} \lambda_j(T_{W_n}) \text{ for all } j$$

- For any convergent graph sequence, the eigenvalues of the graph converge to those of the graphon

Borgs-Chayes-Lovász-Sós-Vesztergombi, *Convergent Sequences of Dense Graphs II. Multiway Cuts and Statistical Physics,*

- For a convergent graph sequence, eigenvalues of the graph converge to those of the limit graphon



- Convergence holds in the sense that $\Rightarrow \exists\, n_0$ s.t. for all $n > n_0$, $\left|\frac{\lambda_j(\mathbf{S}_n)}{n} - \lambda_j(T_{\mathbf{W}})\right| < \epsilon\,, \epsilon > 0$
- But n_0 will be different for each j. Eigenvalue convergence is not uniform

The Graphon Shift Operator Induces a Transform

- The graphon shift operator can be rewritten as

$$(T_W \phi)(v) = \sum_{j=0}^{\infty} \lambda_j \varphi_j(v) \int_0^1 \varphi_j(u) X(u) du$$

- Integral terms correspond to inner products $\langle X, \varphi_j \rangle$ between the signal and the eigenfunctions

- Moreover, the eigenfunctions form a complete orthonormal basis of $L^2([0,1])$

- Thus, the inner products can provide a complete representation of the signal on the graphon basis

- That change of basis is called the graphon Fourier Transform

Definition (Graphon Fourier transform)

The graphon Fourier transform (WFT) of a graphon signal X is defined as a functional $\hat{X} = \text{WFT}(X)$ with continuous input X and discrete output

$$\hat{X}_j = \hat{X}(\lambda_j) = \int_0^1 X(u)\varphi_j(u)du$$

with $\{\lambda_j\}_{j\in\mathbb{Z}/\{0\}}$ the eigenvalues and $\{\varphi_j\}_{j\in\mathbb{Z}/\{0\}}$ the eigenfunctions of T_W

- The eigenvalues λ_j are countable $\Rightarrow$ The graphon Fourier transform $\hat{X}$ can always be defined

Definition (Inverse graphon Fourier transform)

The inverse graphon Fourier transform (iWFT) of a graphon Fourier transform $\hat{X}$ is defined as

$$\text{iWFT}(\hat{X}) = \sum_{j \in \mathbb{Z}/\{0\}} \hat{X}(\lambda_j)\varphi_j = X$$

with $\{\lambda_j\}_{j\in\mathbb{Z}/\{0\}}$ the eigenvalues and $\{\varphi_j\}_{j\in\mathbb{Z}/\{0\}}$ the eigenfunctions of T_W

- Eigenfunctions $\{\varphi_j\}_{j\in\mathbb{Z}/\{0\}}$ are orthonormal. The iWFT is a proper inverse of the WFT

The GFT converges to the WFT

- We discuss the convergence of the GFT to the WFT for graph sequences that converge to graphons.
- This need us to review convergence of eigenvectors and eigenvalues of graph sequences

- Graphon FT, $\text{WFT}(W, X)$ is the eigenspace projection $\Rightarrow \hat{X}_j = \hat{X}(\lambda_j) = \int_0^1 X(u)\, \varphi_j(u)\, du$

- Graph FTs, $\text{GFT}(G_n, \mathbf{x}_n)$ are the eigenspace projections $\Rightarrow \hat{x}_n(j) = \hat{x}_n(\lambda_{nj}) = \sum_{i=1}^{n} x_n(i)\, \mathbf{v}_{nj}(i)$

- Graph signal sequence $(G_n, \mathbf{x}_n)$ converges to graphon signal (W, X) $\Rightarrow$ Conjecture GFT convergence

$$\text{GFT}(G_n, \mathbf{x}_n) \to \text{WFT}(W, X)$$

- Eigenvalue convergence holds $\Rightarrow \lambda_{nj} \to \lambda_j$. Conjecture is reasonable GFT convergence should hold

- Graphon FT, WFT(W, X) is the eigenspace projection $\Rightarrow \hat{X}_j = \hat{X}(\lambda_j) = \int_0^1 X(u)\,\varphi_j(u)\,du$

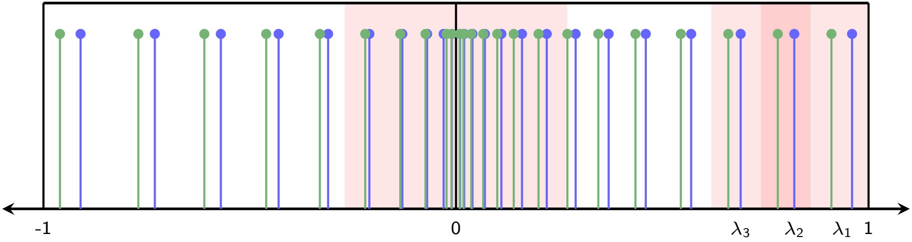
- Graph FTs, GFT$(G_n, \mathbf{x}_n)$ are the eigenspace projections $\Rightarrow \hat{x}_n(j) = \hat{x}_n(\lambda_{nj}) = \sum_{i=1}^{n} \mathbf{x}_n(i)\,\mathbf{v}_{nj}(i)$

- Alas, this conjecture is wrong $\Rightarrow$ GFT convergence to the WFT does not hold in general

$$\text{GFT}(G_n, \mathbf{x}_n) \not\to \text{WFT}(W, X)$$

- GFT and WFT are projections on eigenvectors and eigenfunctions. Not eigenvalues

- Convergence of two eigenvectors depends on how close the eigenvalues of other eigenvectors are
- Eigenvalues accumulate around $\lambda = 0$. They all converge. But different eigenvalues are close
- It makes the eigenvectors slow to converge $\Rightarrow$ They all converge but convergence is not uniform



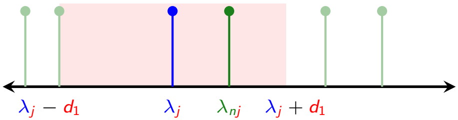
- Consider eigenvalues λ_j of graphon W and λ_{nj} of graph G_n with the same index j

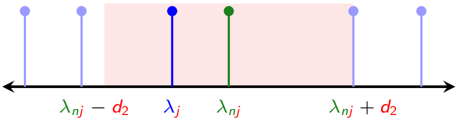
$\Rightarrow$ Compare graphon eigenvalue λ_j to the closest graph eigenvalue other than λ_{nj}

$\Rightarrow$ Compare graph eigenvalue λ_{ni} to the closest graphon eigenvalue other than λ_j

$$d(\lambda_j, \lambda_{nj}) = \min\left(d_1 = \min_{i \neq j} \left| \lambda_j - \lambda_{ni} \right|,\ d_2 = \min_{i \neq j} \left| \lambda_{nj} - \lambda_i \right| \right)$$

$\Rightarrow$ The minimum of these two is the eigenvalue margin $d(\lambda_j, \lambda_{nj})$ for the eigenvalue pair $(\lambda_j, \lambda_{nj})$





Theorem (Davis-Kahan)

Given graphon W and graphon W_{G_n} induced by graph G_n we consider graphon eigenvalue λ_j and graph eigenvalue λ_{nj}. The distance between the associated eigenfunctions is bounded by

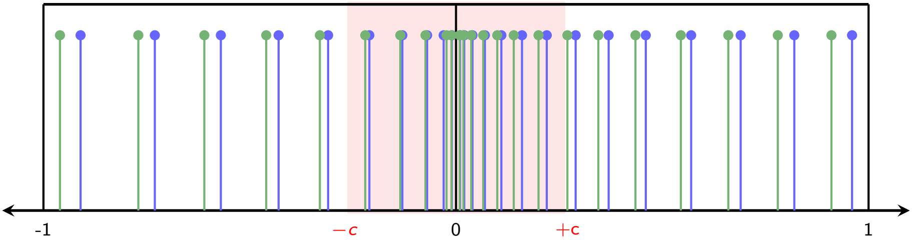
$$\|\varphi_j - \varphi_{nj}\| \leq \frac{\pi}{2} \frac{\|W - W_{G_n}\|}{d(\lambda_j, \lambda_{nj})}$$

where $d(\lambda_j, \lambda_{nj})$ is the eigenvalue margin for the eigenvalue pair $(\lambda_j, \lambda_{nj})$

- Graph eigenvectors converge to graphon eigenfunctions if graph sequence converges to graphon
- When the distance to other eigenvalues decreases, the distance between eigenvectors increases

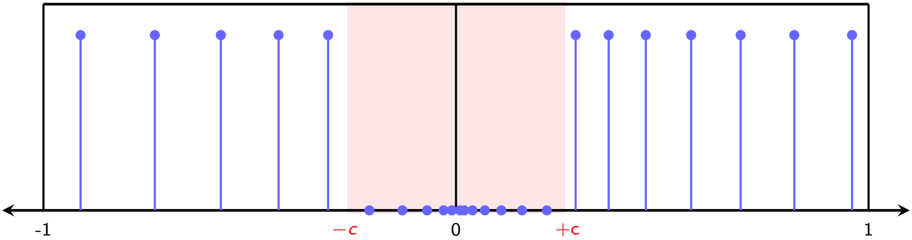
The GFT Does Not Converge to the WFT

- For eigenvalues close to 0 the margin $d(\lambda_j, \lambda_{nj})$ vanishes $\Rightarrow$ There are infinite eigenvalues in $[-c, c]$
- Thus for any n and $\epsilon > 0$ we have some j for which $\Rightarrow \frac{\pi}{2}\frac{\|W - G_n\|}{d(\lambda_j, \lambda_{nj})} > \epsilon$
- Opposite of a convergence claim. $\Rightarrow$ For any $\epsilon > 0$, all $n > n_0$, and j $\Rightarrow \frac{\pi}{2}\frac{\|W - G_n\|}{d(\lambda_j, \lambda_{nj})} \leq \epsilon$

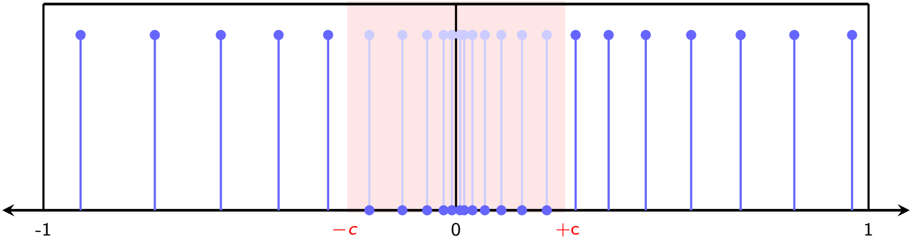


Definition (Graphon bandlimited signals)

A graphon signal (W, X) is c-bandlimited, with bandwith $c \in (0, 1]$, if $\hat{X}(\lambda_j) = 0$ for all $|\lambda_j| < c$.



- Just to emphasize the simplicity of this definition consider a graphon signal that is Not-Bandlimited
- To make it bandlimited it suffices for us to nullify all of the WFT components in the interval $(-c, c)$



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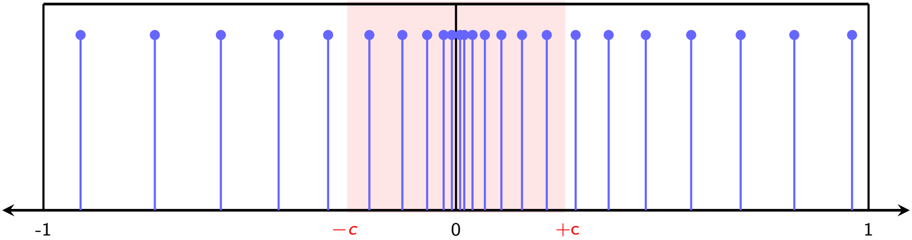


Theorem (GFT convergence for graphon bandlimited signals)

Let $(G_n, \mathbf{x}_n)$ be a sequence of graph signals converging to the c-bandlimited graphon signal (W, X).

There exists a sequence of permutations π_n such that

$$\text{GFT}\Big(\pi_n(G_n), \pi_n(\mathbf{x}_n)\Big) \to \text{WFT}\Big(W, X\Big)$$

Proof: See course webpage https://gnn.seas.upenn.edu/lectures/lecture-9/ ∎

Theorem (iGFT convergence for graphon bandlimited signals)

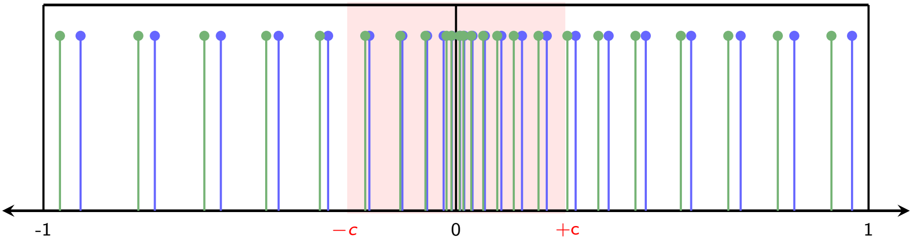
Let $(G_n, \hat{\mathbf{x}}_n)$ be a sequence of GFTs converging to the WFT (W, X). The WFT is associated to a c-bandlimited graphon signal. There exists a sequence of permutations $\{\pi_n\}$ such that

$$\pi_n\Big(\text{iGFT}(\hat{\mathbf{x}}_n)\Big) \to \text{iWFT}\Big(\hat{X}\Big).$$

Proof: See course webpage https://gnn.seas.upenn.edu/lectures/lecture-9/ ■

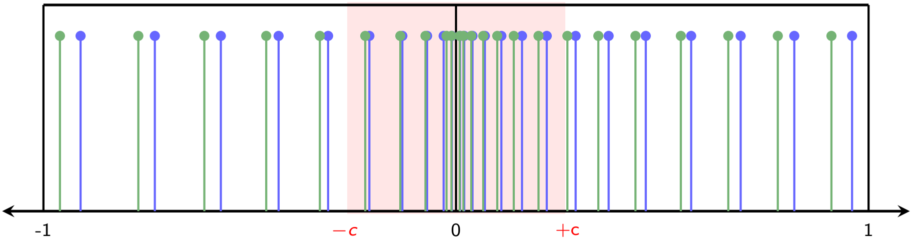
- Convergence of GFT depends on convergence of graph eigenvalues to graphon eigenvalues

- As the number of nodes n grows, the eigenvalues of G_n converge to the eigenvalues of W.



Graph Fourier Transform Convergence for Bandlimited Signals

- However, for large $|j|$ the graph and graphon eigenvalues become difficult to tell apart
- Therefore, the GFT only converges to the WFT for graphon bandlimited signals



Graphon Filters

- We define graphon filters and prove their frequency response, which is independent of the graphon.

- Apply the Graphon shift operator recursively to create the graphon diffusion sequence

$$\left(T_{\mathrm{W}}^{(k)} X \right)(v) \;=\; \int_0^1 \mathrm{W}(u,v) \left(T_{\mathrm{W}}^{(k-1)} X \right)(u)\, du \qquad T_{\mathrm{W}}^{(0)} X = X$$

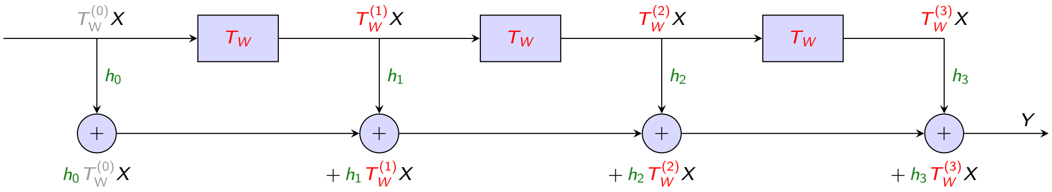
- A graphon filter of order K is defined by the filter coefficients h_k and produces outputs as per

$$Y(v) \;=\; \sum_{k=1}^{K} h_k \left(T_{\mathrm{W}}^{(k)} X \right)(v) \;=\; (T_H X)(v)$$

- A linear combination of the elements of the diffusion sequence modulated by coefficients h_k

- A graphon filter has the same algebraic structure of a graph filter $\Rightarrow Y(v) = \sum_{k=1}^{K} h_k \left(T_W^{(k)} X \right)(v)$

- Only difference is a change of shift operator $\Rightarrow T_W X \ : \ (T_W)X(v) \ = \ \int_0^1 W(u,v)\, X(u)\, du$



⇒ WFTs of input signal ⇒ $\hat{X}_j = \int_0^1 X(u)\varphi_j(u)du$ ⇒ WFT of output ⇒ $\hat{Y}_j = \int_0^1 Y(u)\varphi_j(u)du$

Theorem (Graph frequency representation of graphon filters)

Given a graphon filter T_{H} with coefficients h_k, the components of the graphon Fourier transforms of the input and output signals are related by

$$\hat{Y}_j = \sum_{k=0}^{K} h_k \lambda_j^k \hat{X}_j$$

- The same polynomial that defines the filter but with the eigenvalue λ_i as a variable

Proof: See course webpage https://gnn.seas.upenn.edu/lectures/lecture-9/ ■

- Graphon filters are pointwise in the WFT domain $\Rightarrow \hat{Y}_j = \sum_{k=0}^{K} h_k \lambda_j^k \hat{X}_j = h(\lambda_j)\, \hat{X}_j$

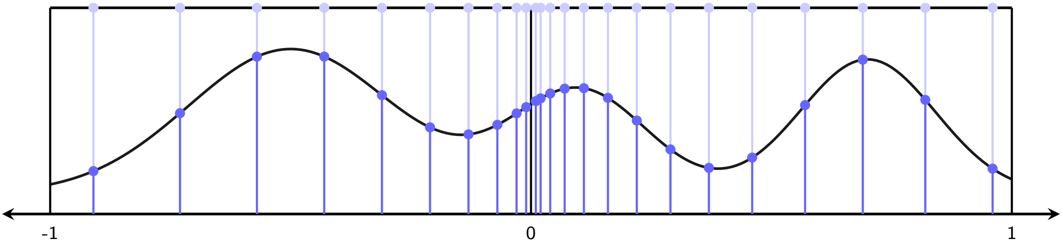
Definition (Frequency response of a graphon filter)

Given a graphon filter with coefficients $\mathrm{h} = \{h_k\}_{k=1}^{\infty}$ the frequency response is the polynomial

$$h(\lambda) = \sum_{k=0}^{\infty} h_k \lambda^k$$

- This is also the exact same definition of the frequency response of a graph filter with coefficients h_k

- The frequency response of a graphon filter and a graph filter with the same coefficients are the same
- Graphon filter instantiates graphon eigenvalues. Graph filter instantiates graph eigenvalues
- If graph sequence converges to a graphon eigenvalues converge $\Rightarrow$ The filter transfers



- The frequency response of a graphon filter and a graph filter with the same coefficients are the same
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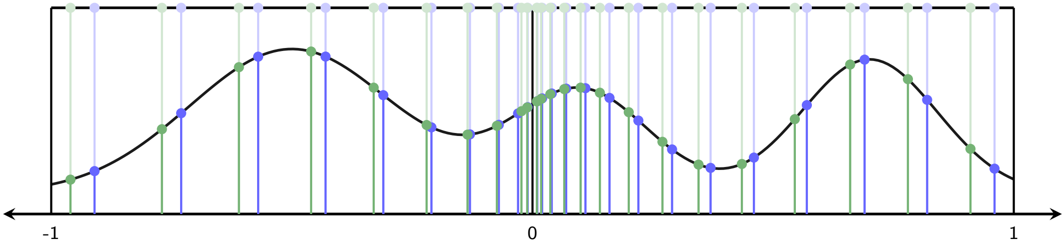
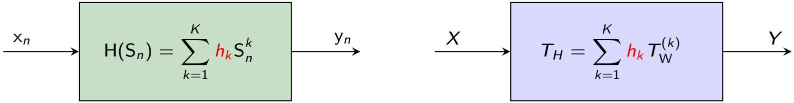


Convergence of Graph Filters in the Spectral Domain

- Convergence of graph filter sequences towards graphon filters for convergent graph signal sequences

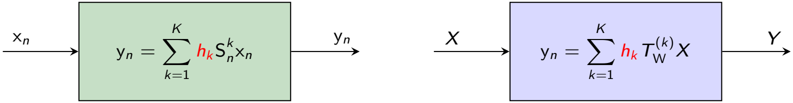
- Given coefficients h_k consider a graph filter sequence and a graphon filter with the same coefficients



- Does the graph filter sequence converge to the graphon filter? $\Rightarrow$ Not the most pertinent question

$\Rightarrow$ Filter convergence is important inasmuch as it implies convergence of filter outputs

- Given coefficients h_k consider a graph filter sequence and a graphon filter with the same coefficients



- Consider a convergent sequence of graph signals $(G_n, \mathbf{x}_n) \to (W, X)$

  $\Rightarrow$ Input graph signal $\mathbf{x}_n$ to graph filter $\mathbf{H}(\mathbf{S}_n)$ to produce output graph signal $\mathbf{y}_n$

  $\Rightarrow$ Input graphon signal X to graphon filter T_H to produce output graphon signal Y

- The graph signal sequence $(G_n, \mathbf{y}_n)$ converges to the graphon signal (W, Y) under some conditions

- Given filter coefficients h_k we have five polynomials which are the same except for their variables

- Two polynomials are representations in the node domain

$\Rightarrow$ The graph filter sequence defined on variable $\mathbf{S}_n$ $\Rightarrow$ $\mathbf{H}(\mathbf{S}_n) = \sum_{k=1}^{K} h_k \mathbf{S}_n^k$

$\Rightarrow$ The graphon filter defined on variable $T_{\mathbf{W}}$ $\Rightarrow$ $T_H = \sum_{k=1}^{K} h_k T_{\mathbf{W}}^{(k)}$

- Given filter coefficients h_k we have five polynomials which are the same except for their variables

- Three polynomials are representations in the spectral domain

$\Rightarrow$ The frequency response of the graph and graphon filters with variable λ $\Rightarrow \tilde{h}(\lambda) = \sum_{k=1}^{K} h_k \lambda^{(k)}$

$\Rightarrow$ The frequency representation of the graph filters with variable λ_{nj} $\Rightarrow \tilde{h}(\lambda_{nj}) = \sum_{k=1}^{K} h_k \lambda_{nj}^{(k)}$

$\Rightarrow$ The frequency representation of the graphon filter with variable λ_j $\Rightarrow \tilde{h}(\lambda_j) = \sum_{k=1}^{K} h_k \lambda_j^{(k)}$

$\Rightarrow$ Frequency representation of graph filters $\Rightarrow$ $\tilde{h}(\lambda_{nj}) = \sum_{k=1}^{K} h_k \lambda_{nj}^k$

$\Rightarrow$ Frequency representation of graphon filter $\Rightarrow$ $\tilde{h}(\lambda_j) = \sum_{k=1}^{K} h_k \lambda_j^k$

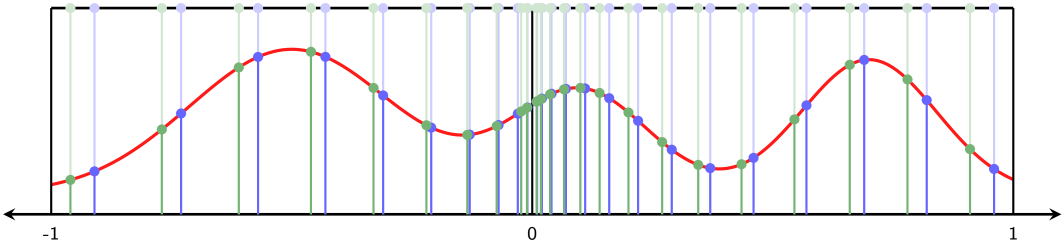
Theorem (Convergence of graph filter sequences in the frequency domain)

Consider filter coefficients h_k generating a sequence of graph filters $\mathrm{H}(\mathrm{S}_n)$ supported on the graph sequence G_n and a graphon filter T_H supported on the graphon W. If $G_n \to W$

$$\lim_{n \to \infty} \tilde{h}(\lambda_{nj}) = \tilde{h}(\lambda_j)$$

Frequency Domain Convergence is Not Much

- Graph filter GFT representations converge to graphon filter WFT representation $\Rightarrow \lim_{n\to\infty} \tilde{h}(\lambda_{nj}) = \tilde{h}(\lambda_j)$
- This is true because eigenvalues converge and the frequency responses are the same
- This is not much to say $\Rightarrow$ GFT and WFT are representations. $\Rightarrow$ Filters operate in the node domain

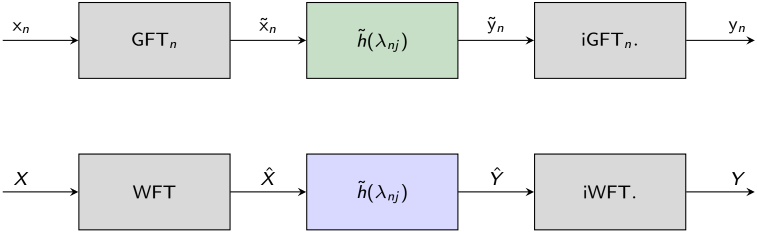


Convergence of Graph Filters in the Node Domain

- We leverage spectral domain convergence to prove convergence of graph filters in the node domain

$\Rightarrow$ Provides a first approach to the study of transferability of graph filters

- To prove convergence in the node domain we can go to the frequency domain and back



- Frequency representation of graph filters converge to frequency representation of graphon filter

$\Rightarrow$ But the GFT and the iGFT do not converge $\Rightarrow$ Unless the signals are graphon bandlimited

- Input graph signal sequence $(G_n, \mathbf{x}_n)$ $\Rightarrow$ Generates output sequence $(G_n, \mathbf{y}_n)$ with $\mathbf{y}_n = \mathbf{H}(\mathbf{S}_n)\mathbf{x}_n$
- Input graphon signal (W, X) $\Rightarrow$ Generates output signal (W, Y) with $Y = T_H X$

Theorem (Graph filter convergence for bandlimited inputs)

Given convergent graph signal sequence $(G_n, \mathbf{x}_n) \to (W, X)$ and filters $\mathbf{H}(\mathbf{S}_n)$ and T_H generated by the same coefficients h_k. If the input signals are c-bandlimited

$$(\mathbf{G}_n, \mathbf{y}_n) \to (\mathbf{W}, Y)$$

The sequence of output graph signals converges to the output graphon signal

- Convergence for bandlimited input is easy. Also weak. Therefore cheap. A stronger result is possible

- Lipschitz graphon filters are filters with frequency responses that are Lipschitz in $[-1, 1]$

$$\Big| h(\lambda_1) - h(\lambda_2) \Big| \;\leq\; L \Big| \lambda_1 - \lambda_2 \Big|, \quad \text{for all } \lambda_1, \lambda_2 \in [0, 1]$$

- Claim convergence of graph filter sequence, despite lack of convergence of the GFT and the iGFT

Theorem (Graph filter convergence for Lipschitz continuous filters)

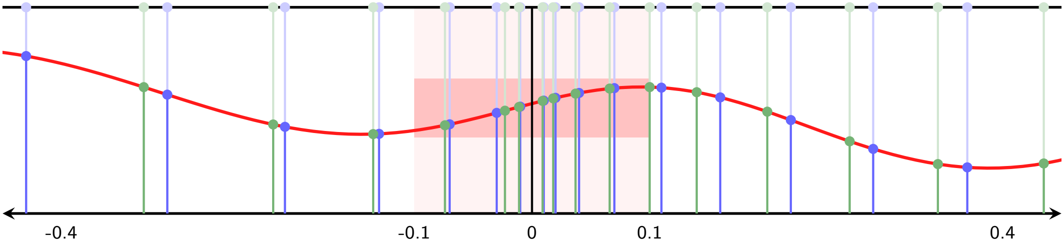
Given convergent graph signal sequence $(G_n, \mathrm{x}_n) \to (W, X)$ and filters $\mathrm{H}(\mathrm{S}_n)$ and T_H generated by the same coefficients h_k. If the frequency response $\tilde{h}(\lambda)$ is Lipschitz

$$(\mathrm{G}_n, \mathrm{y}_n) \to (\mathrm{W}, Y)$$

The sequence of output graph signals converges to the output graphon signal

Proof: See course webpage https://gnn.seas.upenn.edu/lectures/lecture-10/ ■

- The challenge of filter convergence comes from the accumulation of eigenvalues around $\lambda = 0$
- Which causes complications with eigenvector convergence.
- Lipschitz continuity renders the effect void. All components are multiplied by similar numbers

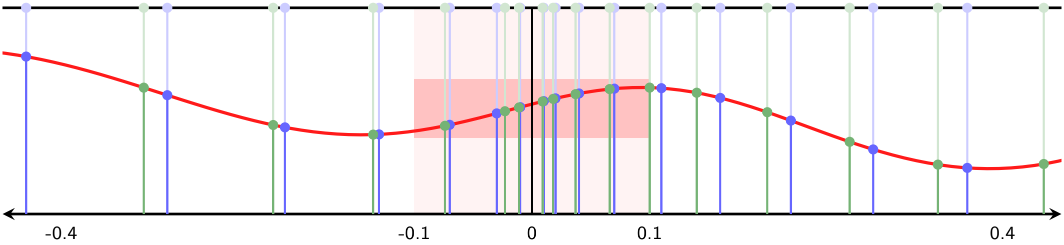


Proof: See course webpage https://gnn.seas.upenn.edu/lectures/lecture-10/ ■

- We identify a fundamental issue $\Rightarrow$ Transferability is counter to discriminability

  $\Rightarrow$ If the filter converges, it can't separate eigenvectors associated to eigenvalues close to $\lambda = 0$

- Characterization is just a limit $\Rightarrow$ Work on a finite-n transference bounding



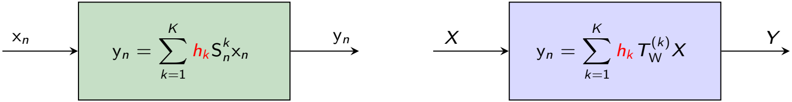
Graphon Filters are Generative Models for Graph Filters

- Graph filters can approximate graphon filters under certain conditions. We discuss them now.

Graphon Filters are Generative Models for Graph Filters

- For a converging graph sequence, graph filters converge asymptotically to graphon filters

- Thus, as n grows, the graph filters become more similar to the graphon filter

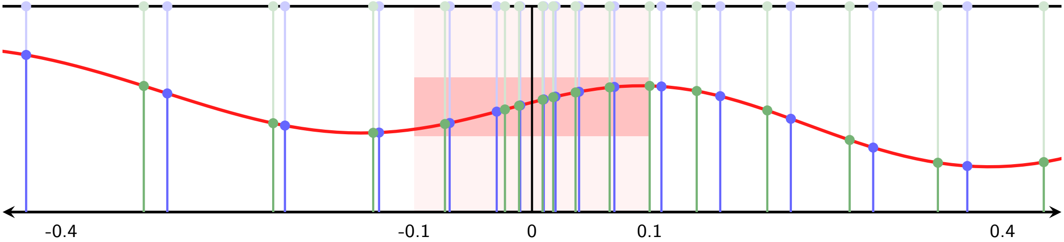


- And we can then use a graph filter as a surrogate for the graphon filter

- We now want to quantify the quality of that approximation for different values of n

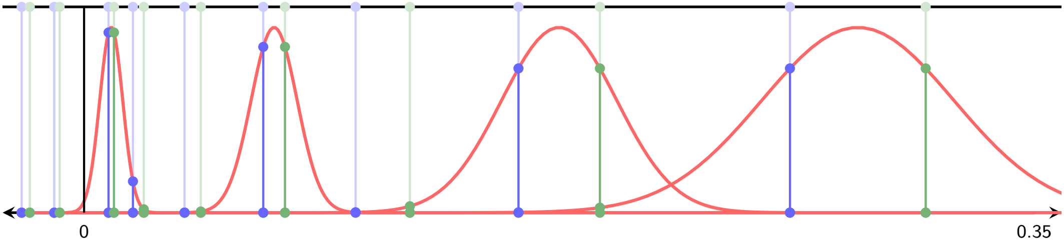
Small Eigenvalues are Hard to Discriminate

- Graphon eigenvalues accumulate at $\lambda = 0$
- Making it hard to match graph eigenvalues to the corresponding graphon eigenvalues if λ is small



Small Eigenvalues are Hard to Discriminate

- Which in turn makes it hard to discriminate consecutive eigenvalues in that range
- If the filter changes rapidly near zero, it may modify the graph and graphon eigenvalues differently
- To obtain good approximations, we must then assume filters do not change much around $\lambda = 0$



- Which in turn makes it hard to discriminate consecutive eigenvalues in that range
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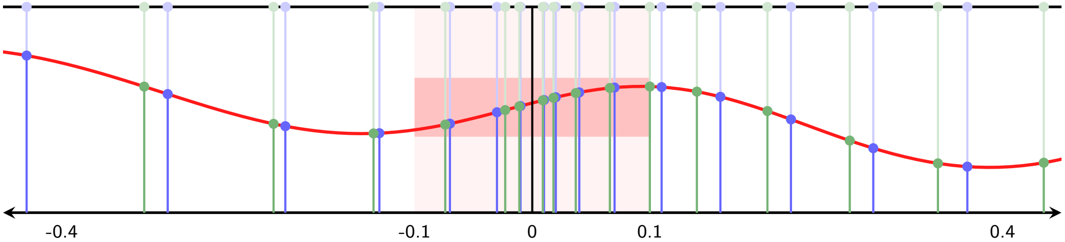
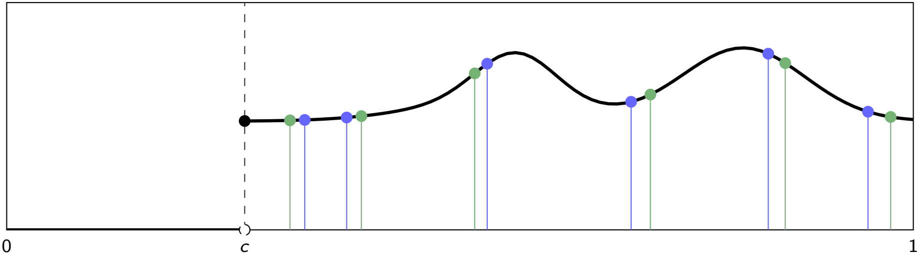


- Graphon eigenvalues tend to zero as the index i grows $\Rightarrow \lim_{i\to\infty} \lambda_i = \lim_{i\to\infty} \lambda_{-i} = 0$

- Low-pass graphon filters must thus be zero for $\lambda < c$. Constant c determines the filter's band.



- The filter removes high frequency components. But low-frequency components are not affected.

(A1) The graphon W is L_1-Lipschitz $\Rightarrow$ For all arguments (u_1, v_1) and (u_2, v_2), it holds

$$\Big| W(u_2, v_2) - W(u_1, v_1) \Big| \leq L_1 \Big(\big| u_2 - u_1 \big| + \big| v_2 - v_1 \big| \Big)$$

(A2) The filter's response is L_2-Lipschitz and normalized $\Rightarrow$ For all λ_1, λ_2 and λ we have

$$\big| \tilde{h}(\lambda_2) - \tilde{h}(\lambda_1) \big| \leq L_2 \big| \lambda_2 - \lambda_1 \big| \quad \text{and} \quad \big| h(\lambda) \big| \leq 1$$

(A3) The graphon signal X is L_3-Lipschitz $\Rightarrow$ For all u_1 and u_2

$$\big| X(u_2) - X(u_1) \big| \leq L_3 \big| u_2 - u_1 \big|$$

- We fix a bandwidth $c > 0$ to separate eigenvalues not close to $\lambda = 0$ and define

(D1) The c-band cardinality of G_n is the number of eigenvalues with absolute value larger than c

$$B_{nc} = \#\Big\{ \lambda_{ni} \;:\; |\lambda_{ni}| > c \Big\}$$

(D2) The c-eigenvalue margin of graph G_n is the

$$\delta_{nc} = \min_{i, j \neq i} \Big\{ |\lambda_{ni} - \lambda_j| \;:\; |\lambda_{ni}| > c \Big\}$$

- Where λ_{ni} are eigenvalues of the shift operator S_n and λ_j are eigenvalues of graphon W

Theorem (Graphon filter approximation by graph filter for low-pass filters)

Consider a graphon filter $Y = \Phi(X; h, W)$ and a graph filter $y_n = \Phi(x_n; h, S_n)$ instantiated from Y. With Definitions **(D1)** - **(D2)**, Assumptions **(A1)** - **(A3)**, and

(A4) $h(\lambda)$ is zero for $|\lambda| < c$

The difference between Y and $Y_n = \Phi(X_n; h, W_n)$ (graph filter induced by y_n) is bounded by

$$\|Y - Y_n\|_{L_2} \leq \sqrt{L_1}\left(L_2 + \frac{\pi n_c}{\delta_{nc}}\right) n^{-\frac{1}{2}} \|X\|_{L_2} + \frac{L_3}{\sqrt{3}} n^{-\frac{1}{2}}$$

Proof: See course webpage https://gnn.seas.upenn.edu/lectures/lecture-10/ ■

- High-pass filters have null frequency response for $|\lambda| > c$, removing low-frequency components
- Moreover, we consider filters that have low variability around $\lambda = 0$

- This makes it easier to match graph eigenvalues to graphon eigenvalues around $\lambda = 0$

Theorem (Graphon filter approximation by graph filter for high-pass filters)

Consider a graphon filter $Y = \Phi(X; h, W)$ and a graph filter $y_n = \Phi(x_n; h, S_n)$ instantiated from Y. With Definitions **(D1)** - **(D2)**, Assumptions **(A1)** - **(A3)**, and

(A4) $h(\lambda)$ is zero for $|\lambda| > c$

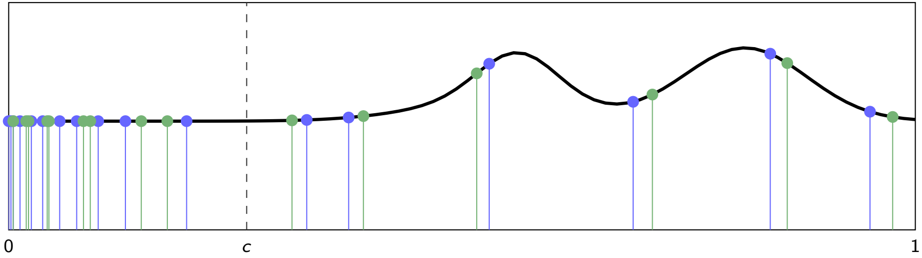
The difference between Y and $Y_n = \Phi(X_n; h, W_n)$ (graph filter induced by y_n) is bounded by

$$\|Y - Y_n\|_{L_2} \leq L_2 c \|X\|$$

Proof: See course webpage https://gnn.seas.upenn.edu/lectures/lecture-10/ ■

- Filter response has low variability for $|\lambda| < c$. Where the eigenvalues of the graphon accumulate

- For $|\lambda| > c$, graphon eigenvalues are countable. And easier to match to those of the graph



- A Lipschitz filter with variable band is the composition of a low-pass filter and a high-pass one

Theorem (Graphon filter approximation by graph filter)

Consider a graphon filter $Y = \Phi(X; h, W)$ and a graph filter $y_n = \Phi(x_n; h, S_n)$ instantiated from Y. With Definitions **(D1)** - **(D2)**, Assumptions **(A1)** - **(A3)**, and

(A4) $h(\lambda)$ has low variability for $|\lambda| < c$

The difference between Y and $Y_n = \Phi(X_n; h, W_n)$ (graph filter induced by y_n) is bounded by

$$\|Y - Y_n\|_{L_2} \leq \sqrt{L_1}\left(L_2 + \frac{\pi n_c}{\delta_{nc}}\right) n^{-\frac{1}{2}} \|X\|_{L_2} + \frac{L_3}{\sqrt{3}} n^{-\frac{1}{2}} + L_2 c \|X\|$$

- Filter with variable band is the sum of an L_2-Lipschitz filter $h_1(\lambda)$ with $h_1(\lambda) = 0$ for $|\lambda| < c$
- And a high-pass filter $h_2(\lambda)$ with $h_2(\lambda)$ showing low variability for $|\lambda| < c$ and 0 otherwise
- Thus, by the triangle inequality

$$\|Y - Y_n\|_{L_2} = \|T_{\mathrm{H}}X - T_{\mathrm{H}_n}\|_{L_2} \leq \|T_{\mathrm{H}_1}X - T_{\mathrm{H}_{1_n}}X_n\|_{L_2} + \|T_{\mathrm{H}_2}X - T_{\mathrm{H}_{2_n}}X_n\|_{L_2}$$

- We know the first-term on the right-hand side. It's the bound for low-pass filters
- And the second-term on the right-hand side is the bound for constant filters
- Summing up the two bounds, we then prove our result for Lipschitz filters with variable band

Theorem (Graphon filter approximation by graph filter)

The difference between Y and $Y_n = \Phi(X_n; \mathrm{h}, \mathrm{W}_n)$ (graph filter induced by y_n) is bounded by

$$\|Y - Y_n\|_{L_2} \leq \sqrt{L_1}\left(L_2 + \frac{\pi n_c}{\delta_{nc}}\right) n^{-\frac{1}{2}} \|X\|_{L_2} + \frac{L_3}{\sqrt{3}} n^{-\frac{1}{2}} + L_2 c \|X\|$$

- Bound depends on the filter transferability constant and on the difference between X and X_n
- Transferability constant depends on the graphon via L_1 which also affects the graphon variability
- As n grows, the transferability constant dominates the bound

Filter Response Determines the Approximation Bound

Theorem (Graphon filter approximation by graph filter)

The difference between Y and $Y_n = \Phi(X_n; \mathbf{h}, \mathbf{W}_n)$ (graph filter induced by $\mathbf{y}_n$) is bounded by

$$\|Y - Y_n\|_{L_2} \leq \sqrt{L_1}\left(L_2 + \frac{\pi n_c}{\delta_{nc}}\right) n^{-\frac{1}{2}}\|X\|_{L_2} + \frac{L_3}{\sqrt{3}} n^{-\frac{1}{2}} + L_2 c\|X\|$$

- Transferability constant depends on the filter parameters L_2, n_c and δ_{nc}
- Filter's Lipschitz constant L_2 and filter's band $[c, 1]$ determine variability of the spectral response
- Number of eigenvalues in the passing band has to be limited: $n_c < \sqrt{n}$
- This ensures eigenvalues of $\mathbf{W}_n$ converge to those of $\mathbf{W}$. And thus so does the filter approximation

- We identify a fundamental issue $\Rightarrow$ Good approximations are counter to discriminability

  $\Rightarrow$ Tight approximation bounds require filters with low variability around $\lambda = 0$

  $\Rightarrow$ But then the filter can't discriminate components associated to eigenvalues close to $\lambda = 0$

- That is less of an issue for larger graphs. Filter approximation requires $n_c < \sqrt{n}$

  $\Rightarrow$ As n grows, we can afford a larger number of eigenvalues n_c in the passing band

  $\Rightarrow$ Improving discriminability without penalizing the approximation bound

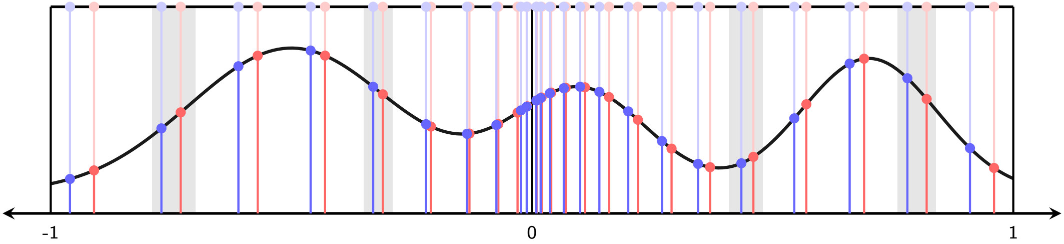
Transferability of Graph Filters: Theorem

- We show that graph filters are transferable across graphs that are drawn from a common graphon

- Have not proven transferability $\Rightarrow$ Have proven that graph filters are close to graphon filters

$\Rightarrow$ Graph G_n with n nodes sampled from graphon W

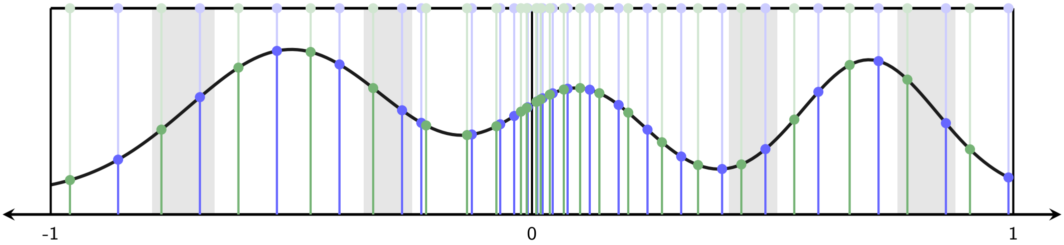
$\Rightarrow$ Have shown that graph filter $\mathrm{H}(\mathrm{S}_n)$ running on G_n is close to the graphon filter T_H



- Transferability means that two different graphs with different number of nodes are close

⇒ Graph G_n and graph G_m with $n \neq m$ nodes. Both sampled from graphon W

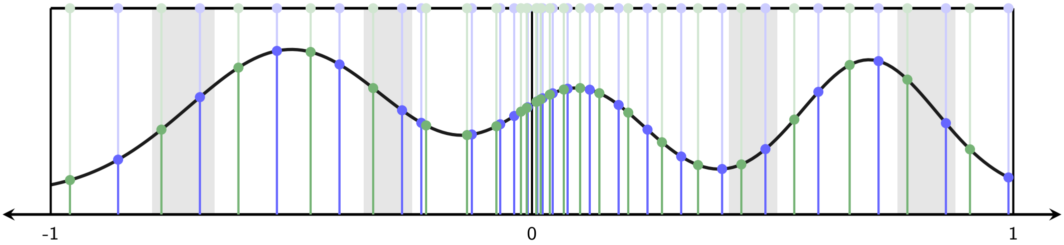
⇒ Want to show that graph filter $\text{H}(\text{S}_n)$ and graph filter $\text{H}(\text{S}_m)$ are close



- But graph filters are close because they are both close to the graphon filter

$\Rightarrow$ Graph filter $\mathrm{H}(\mathrm{S}_n)$ close to graphon filter T_H. Graph filter $\mathrm{H}(\mathrm{S}_m)$ close to graphon filter T_H

$\Rightarrow$ Graph filter $\mathrm{H}(\mathrm{S}_n)$ is close to graph filter $\mathrm{H}(\mathrm{S}_m)$ $\Rightarrow$ This is just the triangle inequality



Running the Same Filter on Different Graphs

- Consider graph signals $(\mathbf{S}_n, \mathbf{x}_n)$ and $(\mathbf{S}_m, \mathbf{x}_m)$ sampled from the graphon signal (W, X)

- Given filter coefficients h_k we process signals on their respective graphs

$\Rightarrow$ Run filter with coefficients h_k on graph S_n to process x_n $\Rightarrow \mathbf{y}_n = \mathbf{H}(\mathbf{S}_n)\mathbf{x}_n = \sum_{k=1}^{K} h_k \mathbf{S}_n^k \mathbf{x}_n$

$\Rightarrow$ Run filter with coefficients h_k on graph S_m to process x_m $\Rightarrow \mathbf{y}_m = \mathbf{H}(\mathbf{S}_m)\mathbf{x}_m = \sum_{k=1}^{K} h_k \mathbf{S}_m^k \mathbf{x}_n$

- Since they have different number of components we compare induced graphon signals Y_n and Y_m

(A1) The graphon W is L_1-Lipschitz $\Rightarrow$ For all arguments (u_1, v_1) and (u_2, v_2), it holds

$$\left| W(u_2, v_2) - W(u_1, v_1) \right| \leq L_1 \Big(\left| u_2 - u_1 \right| + \left| v_2 - v_1 \right| \Big)$$

(A2) The filter's response is L_2-Lipschitz and normalized $\Rightarrow$ For all λ_1, λ_2 and λ we have

$$\left| \tilde{h}(\lambda_2) - \tilde{h}(\lambda_1) \right| \leq L_2 \left| \lambda_2 - \lambda_1 \right| \qquad \text{and} \qquad \left| h(\lambda) \right| \leq 1$$

(A3) The graphon signal X is L_3-Lipschitz $\Rightarrow$ For all u_1 and u_2

$$\left| X(u_2) - X(u_1) \right| \leq L_3 \left| u_2 - u_1 \right|$$

- We fix a bandwidth $c > 0$ to separate eigenvalues not close to $\lambda = 0$ and define

(D1) The c-band cardinality of G_n is the number of eigenvalues with absolute value larger than c

$$B_{nc} = \#\left\{ \lambda_{ni} \ : \ |\lambda_{ni}| > c \right\}$$

(D2) The c-eigenvalue margin of of graph G_n is the

$$\delta_{nc} = \min_{i, j \neq i} \left\{ |\lambda_{ni} - \lambda_j| \ : \ |\lambda_{ni}| > c \right\}$$

- Where λ_{ni} are eigenvalues of the shift operator S_n and λ_j are eigenvalues of graphon W

Theorem (Graph filter transferability)

Consider graph signals $(\mathbf{S}_n, \mathbf{x}_n)$ and $(\mathbf{S}_m, \mathbf{x}_m)$ sampled from graphon signal (W, X) along with filter outputs $\mathbf{y}_n = \mathbf{H}(\mathbf{S}_n)\mathbf{x}_n$ and $\mathbf{y}_m = \mathbf{H}(\mathbf{S}_m)\mathbf{x}_m$. With Assumptions (A1)-(A3) and Definitions (D1)-(D2) the difference norm of the respective graphon induced signals is bounded by

$$\|Y_n - Y_m\| \leq \sqrt{L_1}\left(L_2 + \pi\frac{\max(B_{nc}, B_{mc})}{\min(\delta_{nc}, \delta_{mc})}\right)\left(\frac{1}{\sqrt{n}} + \frac{1}{\sqrt{m}}\right)\|X\| + \frac{2L_3}{\sqrt{3}}\left(\frac{1}{\sqrt{n}} + \frac{1}{\sqrt{m}}\right) + L_2 c\|X\|$$

Proof: See course webpage https://gnn.seas.upenn.edu/lectures/lecture-10/ ■

Transferability of Graph Filters: Remarks

- We present remarks on the transferability theorem of graph filters sampled from a graphon filter

Theorem (Graph filter transferability)

The difference norm of the respective graphon induced signals is bounded by

$$\|Y_n - Y_m\| \leq \sqrt{L_1}\left(L_2 + \pi\frac{\max(B_{nc}, B_{mc})}{\min(\delta_{nc}, \delta_{mc})}\right)\left(\frac{1}{\sqrt{n}} + \frac{1}{\sqrt{m}}\right)\|X\| + \frac{2L_3}{\sqrt{3}}\left(\frac{1}{\sqrt{n}} + \frac{1}{\sqrt{m}}\right) + L_2 c\|X\|$$

Thing 1: A term that comes from the discretization of the graphon signal $\Rightarrow$ Not very important

Thing 2: A term coming from filter variability at eigenvalues $|\lambda| > c$ $\Rightarrow$ The easy components

Thing 3: A term coming from filter variability at eigenvalues $|\lambda| \leq c$ $\Rightarrow$ The difficult components

Theorem (Graph filter transferability)

The difference norm of the respective graphon induced signals is bounded by

$$\|Y_n - Y_m\| \leq \sqrt{L_1}\left(L_2 + \pi\frac{\max(B_{nc}, B_{mc})}{\min(\delta_{nc}, \delta_{mc})}\right)\left(\frac{1}{\sqrt{n}} + \frac{1}{\sqrt{m}}\right)\|X\| + \frac{2L_3}{\sqrt{3}}\left(\frac{1}{\sqrt{n}} + \frac{1}{\sqrt{m}}\right) + L_2 c\|X\|$$

- As $(n, m) \to \infty$ most of the transferability error decreases with the square root of the graph sizes
- We can also afford smaller bandwidth limit c $\Rightarrow$ Transfer filters closer to $\lambda = 0$
- Sharper filter responses (larger Lipschitz constant L_2) $\Rightarrow$ Transfer more discriminative filters

Theorem (Graph filter transferability)

The difference norm of the respective graphon induced signals is bounded by

$$\|Y_n - Y_m\| \ \leq \ \sqrt{L_1}\left(L_2 + \pi\frac{\max(B_{nc}, B_{mc})}{\min(\delta_{nc}, \delta_{mc})}\right)\left(\frac{1}{\sqrt{n}} + \frac{1}{\sqrt{m}}\right)\|X\| + \frac{2L_3}{\sqrt{3}}\left(\frac{1}{\sqrt{n}} + \frac{1}{\sqrt{m}}\right) + L_2 c\|X\|$$

- Graph signals and graphons with rapid variability make filter transference more difficult
- This is because of sampling approximation error $\Rightarrow$ Not fundamental
- The constants can be sharpened with modulo-permutation Lipschitz constants

Theorem (Graph filter transferability)

The difference norm of the respective graphon induced signals is bounded by

$$\|Y_n - Y_m\| \leq \sqrt{L_1}\left(L_2 + \pi\frac{\max(B_{nc}, B_{mc})}{\min(\delta_{nc}, \delta_{mc})}\right)\left(\frac{1}{\sqrt{n}} + \frac{1}{\sqrt{m}}\right)\|X\| + \frac{2L_3}{\sqrt{3}}\left(\frac{1}{\sqrt{n}} + \frac{1}{\sqrt{m}}\right) + L_2 c\|X\|$$

- Filters that are more discriminative are more difficult to transfer

  $\Rightarrow$ True in the part of the bound related to easy components associated with eigenvalues $|\lambda| > c$

  $\Rightarrow$ True in the part of the bound related to difficult components associated with eigenvalues $|\lambda| \leq c$

Theorem (Graph filter transferability)

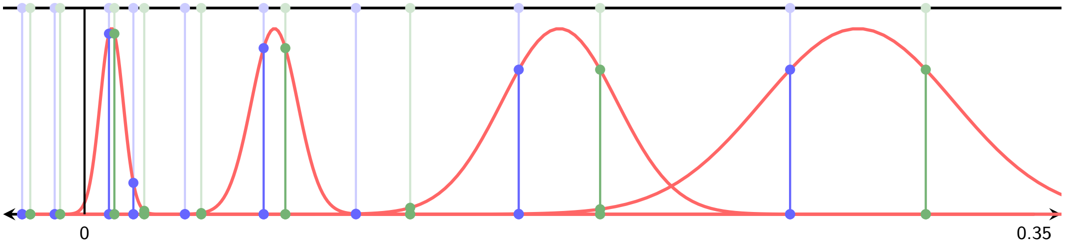
The difference norm of the respective graphon induced signals is bounded by

$$\|Y_n - Y_m\| \leq \sqrt{L_1}\left(L_2 + \pi\frac{\max(B_{nc}, B_{mc})}{\min(\delta_{nc}, \delta_{mc})}\right)\left(\frac{1}{\sqrt{n}} + \frac{1}{\sqrt{m}}\right)\|X\| + \frac{2L_3}{\sqrt{3}}\left(\frac{1}{\sqrt{n}} + \frac{1}{\sqrt{m}}\right) + L_2 c\|X\|$$

- Bound is parametric on the bandwidth c $\Rightarrow$ Different c result in different values for the bound
- Increase c-band cardinality or decrease c-eigenvalue margin $\Rightarrow$ More challenging transferability
- A property of the graphon $\Rightarrow$ Since eigenvalues converge B_{nc} and δ_{nc} converge

Transferability vs Discriminability Non-Tradeoff

- If we fix n and m we observe emergence of a transferability vs discriminability non-tradeoff
- Discriminating around $\lambda = 0$ needs large Lipschitz constant L_2 $\Rightarrow$ Useless transferability bound
- To make transferability and discriminability compatible $\Rightarrow$ Graph Neural Networks



Transferability of GNNs

- We define graphon neural networks and discuss their interpretation as generative models for GNNs
- We show that graph neural networks inherit the transferability properties of graph filters

- Graph filters are transferable $\Rightarrow$ we can expect GNNs to inherit transferability from graph filters

- To analyze GNN transferability, we we first define Graphon Neural Networks (WNNs)

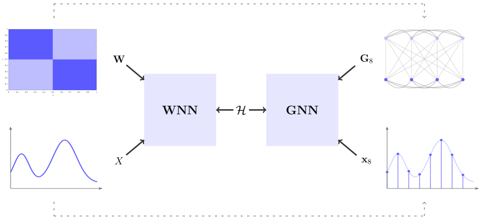
- The lth layer of a WNN composes a graphon convolution with parameters h and a nonlinearity σ

$$X_l^f = \sigma\left(\sum_{g=1}^{F_{l-1}} h_{kl}^{fg} T_W^{(k)} X_{l-1}^g\right)$$

L layers, $1 \leq f \leq F_l$ output features per layer. WNN input is $X_0 = X$. Output is $Y = X_L$

- Can be represented as $Y = \Phi(\mathcal{H}; W; X)$ with coefficients $\mathcal{H} = \{\mathrm{h}_{kl}^{fg}\}_{k,l,f,g}$. Just like the GNN

- As in the GNN map $\Phi(\mathcal{H}; S; x)$, in the WNN $\Phi(\mathcal{H}; W; X)$, the set $\mathcal{H}$ doesn't depend on the graphon
- Therefore, we can use WNNs to instantiate GNNs $\Rightarrow$ the WNN is a generative model for GNNs



- We will consider GNNs $\Phi(\mathcal{H}; S_n; x_n)$ instantiated from $\Phi(\mathcal{H}; W; X)$ on weighted graphs G_n

$$[S_n]_{ij} = W(u_i, u_j) \qquad [x_n]_i = X(u_i)$$

Sampling a GNN from the WNN

- Consider a graph signal $(\mathbf{S}_n, \mathbf{x}_n)$ sampled from the graphon signal (W, X)

- Given WNN coefficients $\mathcal{H}$ for L layers, width $F_l = F$ for $1 \leq l < L$, and $F_0 = F_L = 1$

  $\Rightarrow$ Run WNN with coefficients $\mathcal{H}$ on graphon W to process X $\Rightarrow Y = \Phi(\mathcal{H}; W, X)$

  $\Rightarrow$ Run GNN with coefficients $\mathcal{H}$ on graph S_n to process x_n $\Rightarrow \mathbf{y}_n = \Phi(\mathcal{H}; S_n, x_n)$

- Since one is a vector and the other a function we consider the induced graphon signal Y_n

(A1) The graphon W is L_1-Lipschitz $\Rightarrow$ For all arguments (u_1, v_1) and (u_2, v_2), it holds

$$\left| W(u_2, v_2) - W(u_1, v_1) \right| \leq L_1 \Big(\left| u_2 - u_1 \right| + \left| v_2 - v_1 \right| \Big)$$

(A2) The filter's response is L_2-Lipschitz and normalized $\Rightarrow$ For all λ_1, λ_2 and λ we have

$$\left| \tilde{h}(\lambda_2) - \tilde{h}(\lambda_1) \right| \leq L_2 \left| \lambda_2 - \lambda_1 \right| \quad \text{and} \quad \left| h(\lambda) \right| \leq 1$$

(A3) The graphon signal X is L_3-Lipschitz $\Rightarrow$ For all u_1 and u_2

$$\left| X(u_2) - X(u_1) \right| \leq L_3 \left| u_2 - u_1 \right|$$

(A4) The nonlinearities σ are normalized Lipschitz and $\sigma(0) = 0$ $\Rightarrow$ For all x and y

$$\left| \sigma(x) - \sigma(y) \right| \leq |x - y|$$

- We fix a bandwidth $c > 0$ to separate eigenvalues not close to $\lambda = 0$ and define

(D1) The c-band cardinality of G_n is the number of eigenvalues with absolute value larger than c

$$B_{nc} = \#\left\{ \lambda_{ni} \ : \ |\lambda_{ni}| > c \right\}$$

(D2) The c-eigenvalue margin of of graph G_n is the

$$\delta_{nc} = \min_{i, j \neq i} \left\{ |\lambda_{ni} - \lambda_j| \ : \ |\lambda_{ni}| > c \right\}$$

- Where λ_{ni} are eigenvalues of the shift operator S_n and λ_j are eigenvalues of graphon W

Theorem (GNN-WNN approximation)

Consider the graph signal (S_n, x_n) sampled from the graphon signal (W, X) along with the GNN output $y_n = \Phi(\mathcal{H}; S_n, x_n)$ and WNN output $Y = \Phi(\mathcal{H}; W, X)$. With Assumptions (A1)-(A4) and Definitions (D1)-(D2) the norm difference $\|Y_n - Y\|$ is bounded by

$$\|Y - Y_n\| \leq LF^{L-1}\sqrt{L_1}\left(L_2 + \pi\frac{B_{nc}}{\delta_{nc}}\right)\left(\frac{1}{\sqrt{n}}\right)\|X\| + \frac{L_3}{\sqrt{3}}\left(\frac{1}{\sqrt{n}}\right) + LF^{L-1}L_2 c\|X\|$$

Proof: See course webpage https://gnn.seas.upenn.edu/lectures/lecture-10/ ■

- The error incurred when using a GNN to approximate a WNN can be upper bounded
- Same comments as for graph and graphon filters apply. With additional dependence on L and F
- Distances between GNNs and WNN can be combined to calculate distance between GNNs
- GNNs $Y_n = \Phi(\mathcal{H}; W_n, x_n)$ and $Y_m = \Phi(\mathcal{H}; W_m, x_m)$ instantiated from WNN $Y = \Phi(\mathcal{H}; W, X)$

$$\|Y_n - Y_m\| = \|Y_n - Y + Y - Y_m\| \leq \|Y_n - Y\| + \|Y - Y_m\|$$

- The inequality follows from the triangle inequality. By which we have proved GNN transferability

Running the Same GNN on Different Graphs

- Consider graph signals $(\mathbf{S}_n, \mathbf{x}_n)$ and $(\mathbf{S}_m, \mathbf{x}_m)$ sampled from the graphon signal (W, X)

- Given GNN coefficients $\mathcal{H}$ for L layers, width $F_l = F$ for $1 \leq l < L$, and $F_0 = F_L = 1$

  $\Rightarrow$ Run GNN with coefficients $\mathcal{H}$ on graph S_n to process x_n $\Rightarrow y_n = \Phi(\mathcal{H}; S_n, x_n)$

  $\Rightarrow$ Run filter with coefficients $\mathcal{H}$ on graph S_m to process x_m $\Rightarrow y_m = \Phi(\mathcal{H}; S_m, x_n)$

- Since they have different number of components we compare induced graphon signals Y_n and Y_m

Penn

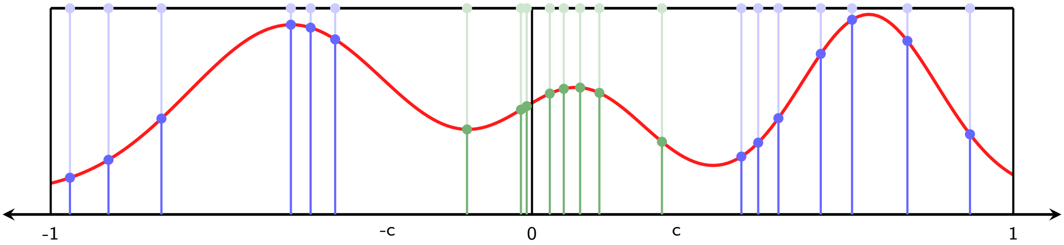
Theorem (GNN transferability)

Consider graph signals $(\mathbf{S}_n, \mathbf{x}_n)$ and $(\mathbf{S}_m, \mathbf{x}_m)$ sampled from graphon signal (W, X) along with GNN outputs $\mathbf{y}_n = \Phi(\mathcal{H}; \mathbf{S}_n, \mathbf{x}_n)$ and $\mathbf{y}_m = \Phi(\mathcal{H}; \mathbf{S}_m, \mathbf{x}_m)$. With Assumptions (A1)-(A4) and Definitions (D1)-(D2) the difference norm of the respective graphon induced signals is bounded by

$$\|Y_n - Y_m\| \leq LF^{L-1}\sqrt{L_1}\left(L_2 + \pi\frac{\max(B_{nc}, B_{mc})}{\min(\delta_{nc}, \delta_{mc})}\right)\left(\frac{1}{\sqrt{n}} + \frac{1}{\sqrt{m}}\right)\|X\| + \frac{L_3}{\sqrt{3}}\left(\frac{1}{\sqrt{n}} + \frac{1}{\sqrt{m}}\right) + LF^{L-1}L_2 c\|X\|$$

- Same comments as in the case of graph filter transferability. With additional dependence on L, F

- The transferability-discriminability trade-off looks the same. But it is helped by the nonlinearities
- At each layer of the GNN, the nonlinearities σ scatter eigenvalues from $|\lambda| \leq c$ to $|\lambda| > c$



- Nonlinearities allows $\downarrow c$ and $\uparrow L_2$ $\Rightarrow$ increasing discriminability while retaining transferability
- For the same level of discriminability, GNNs are more transferable than graph filters