



▶ 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  $\Rightarrow$  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  $\Rightarrow W(u, v) = W(v, u)$ 



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### $\blacktriangleright$ 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 ⇒ The product similarity "graphon"



n = 30 products

n = 50 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



- ▶ Vertices: For an *n*-node graph, sample *n* points  $\{u_1, u_2, ..., u_n\}$  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  $i \in \{1, 2, 3, \dots, n\}$  of the graph
- Edges: Evaluate  $W(u_i, u_j)$  for edge (i, j)
  - $\Rightarrow$  Stochastic: Connect *i* and *j* with an unweighted undirected edge with probability W( $u_i, u_j$ )
  - $\Rightarrow$  Weighted: Connect *i* and *j* with weighted undirected edge with weight W( $u_i, u_j$ )



► Use uniform Graphon



To generate random graphs with the same

Or different number of nodes









Graphon







To generate balanced SBM graphs with the same

Or different number of nodes

n = 20 nodes

n = 20 nodes

n = 40 nodes





Graphon



To generate unbalanced SBM graphs with the same

### Or different number of nodes



n = 20 nodes

n = 20 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





# 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





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



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

## Motifs and Graph Homomorphisms



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• Given motif F and graph G, there are multiple homomorphism functions  $\beta$ 



 $\blacktriangleright$  We define 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

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

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



• 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

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

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

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

 $\blacktriangleright$  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

## Example of Convergent Graph Sequence

- Consider a sequence of random graphs  $\{G_n\}$  sampled from the graphon W. Graphs  $G_n$  have
  - $\Rightarrow$  Labels  $u_i \sim \textit{U}[0,1]$  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







Every undirected graph admits a graphon representation which we call its induced graphon

 $\rightarrow$ 

- Consider a graph  $G = \{\mathcal{V}, \mathcal{E}, S\}$  with  $|\mathcal{V}| = n$  and normalized graph shift operator S
- ▶ Regular partition of the unit interval with *n* subintervals  $\Rightarrow$   $I_i = [(i-1)/n, i/n]$
- ▶ We define the induced graphon  $W_G \Rightarrow W_G(u, v) = [S]_{ij} \mathbb{I}(u \in I_i) \mathbb{I}(v \in I_j)$





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  $X : [0, 1] \rightarrow \mathbb{R}$  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  $(S_n, x_n)$  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  $I_i = [(i-1)/n, i/n]$ 
  - $\Rightarrow$  Induced signal  $X_G(u) = x_i \mathbb{I}(u \in I_i)$
  - $\Rightarrow$   $W_G$  is the graphon induced by the graph  $G \Rightarrow W_G(u, v) = [S]_{ij} \mathbb{I}(u \in I_i) \mathbb{I}(v \in I_j)$







### Definition (Convergent sequences of graph signals)

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

$$t(F, G_n) \rightarrow t(F, W),$$
 and  $X_{\pi_n(G_n)} - X \Big|_{L^2} \rightarrow 0$ 

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

▶ The permutation is used here to make the convergence definition independent of labels

**•** To enable comparison of the vector  $x_n$  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  $\Rightarrow T_W : L^2([0,1]) \rightarrow L^2([0,1])$
- ▶ When applied to the graphon signal X, the operator  $T_W$  produces the signal  $T_W X$  with values

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

- ▶ 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  $\Rightarrow (T_WX)(v) = \int_0^1 W(u,v)X(u) du$ 

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

$$(T_{W}\varphi)(v) = \int_{0}^{1} W(u, v)\varphi(u) \, du = \lambda \varphi(v)$$

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

• 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  $T_W$ 

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

• More or less the same as the eigenvector decomposition  $\Rightarrow S = V \wedge V^H = \sum_{i=1}^{\infty} \lambda_i \mathbf{v}_i \mathbf{v}_i^T$ 



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

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





- 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  $|\lambda_i| \ge c$  is finite  $\Rightarrow \# \left\{ \lambda_i : |\lambda_i| \ge c \right\} = n_c < \infty$
- ▶ 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

$$\lim_{n\to\infty}\frac{\lambda_j(\mathsf{S}_n)}{n} = \lambda_j(\mathsf{T}_\mathsf{W}) = \lim_{n\to\infty}\lambda_j(\mathsf{T}_{\mathsf{W}_n}) \text{ for all } j$$

### ▶ 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  $n > n_0$ ,  $\left| \frac{\lambda_j(S_n)}{n} - \lambda_j(T_W) \right| < \epsilon, \epsilon > 0$ 

**b** But  $n_0$  will be different for each *j*. Eigenvalue convergence is not uniform



The graphon shift operator can be rewritten as

$$(T_{\mathsf{W}}\phi)(\boldsymbol{v}) = \sum_{j=0}^{\infty} \lambda_j \varphi_j(\boldsymbol{v}) \int_0^1 \varphi_j(\boldsymbol{u}) X(\boldsymbol{u}) d\boldsymbol{u}$$

- ▶ 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  $\hat{X}$  =

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  $\lambda_i$  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

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

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

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, 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(
$$G_n, x_n$$
) are the eigenspace projections  $\Rightarrow \hat{x}_n(j) = \hat{x}_n(\lambda_{nj}) = \sum_{i=1}^n x_n(i) v_{nj}(i)$ 

• Graph signal sequence  $(G_n, x_n)$  converges to graphon signal  $(W, X) \Rightarrow$  Conjecture GFT convergence

 $GFT(G_n, x_n) \rightarrow WFT(W, X)$ 

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



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

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

 $GFT(G_n, x_n) \not\rightarrow WFT(W, X)$ 

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

## Convergence to Graphon Eigenvectors

- 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  $\lambda_j$  of graphon W and  $\lambda_{nj}$  of graph  $G_n$  with the same index j
  - $\Rightarrow$  Compare graphon eigenvalue  $\lambda_j$  to the closest graph eigenvalue other than  $\lambda_{nj}$
  - $\Rightarrow$  Compare graph eigenvalue  $\lambda_{ni}$  to the closest graphon eigenvalue other than  $\lambda_j$

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

 $\Rightarrow$  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  $\lambda_j$  and graph eigenvalue  $\lambda_{nj}$ . 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



Thus for any *n* and 
$$\epsilon > 0$$
 we have some *j* for which  $\Rightarrow \frac{\pi}{2} \frac{\|W - G_n\|}{d(\lambda_i, \lambda_{nj})} > \epsilon$ 

• 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  $\hat{X}(\lambda_i) = 0$  for all  $|\lambda_i| < c$ .





- 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  $(G_n, x_n)$  be a sequence of graph signals converging to the *c*-bandlimited graphon signal (W, X).

There exists a sequence of permutations  $\pi_n$  such that

$$\mathsf{GFT}\Big(\pi_n(G_n),\pi_n(\mathsf{x}_n)\Big) \rightarrow \mathsf{WFT}\Big(W,X\Big)$$

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



## Theorem (iGFT convergence for graphon bandlimited signals)

Let  $(G_n, \hat{x}_n)$  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

$$\pi_n(\operatorname{iGFT}(\hat{\mathbf{x}}_n)) \rightarrow \operatorname{iWFT}(\hat{\mathbf{X}}).$$

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.





- 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

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

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

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

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





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

Theorem (Graph frequency representation of graphon filters)

Given a graphon filter  $T_{\rm H}$  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  $\lambda_i$  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  $h = {h_k}_{k=1}^{\infty}$  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 ⇒ The filter transfers



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