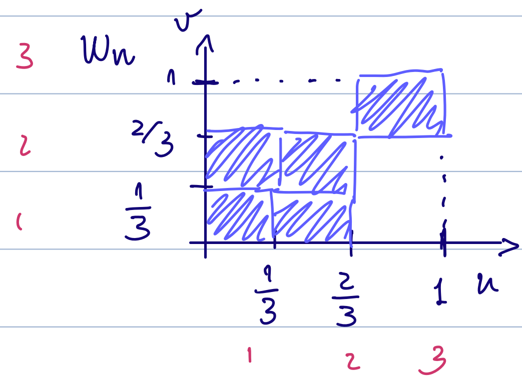
Lecture 15 EN.553.744 Prof. Luana Ruiz

Define $W_n(u,v) = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} \, \mathbb{I}(u \in I_i) \, \mathbb{I}(v \in I_j)$

the "induced graphon"

E.g.:

$$A_n = \begin{array}{c} \\ 1 \\ 2 \\ 3 \end{array} \begin{array}{c} \begin{array}{ccc} 1 & 2 & 3 \end{array} \\ \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \end{array}$$



Using transformation (*), we can represent both G_n and G_m as kernels on $[0,1]^2$, so they are compatible objects. But now we need a notion of cut norm for kernels.

Cut norm: Let W be a kernel in $[0,1]^2$. Its cut norm is defined as:

$$\|W\|_{\square} = \sup_{S,T \subseteq [0,1]} \left| \iint_{S \times T} W(u,v) \, du\, dv \right|$$

We're not done yet! We need to take into account "node relabelings" (permutations of $I_1, I_2, \ldots$).

So for two kernels (graphons), we define the cut metric:

$$\delta_\square (W, W') = \inf_{\phi} \| W^{\phi} - W' \|_\square$$

where $W^{\phi}(u,v) = W(\phi(u), \phi(v))$ and ϕ are measure-preserving bijections

Hence $\delta_\square (G_n, G_m) = \delta_\square (W_n, W_m)$

Sequences of graphs $(G_n)_n$ converging to a graphon W also converge in the cut metric!

$$G_n \xrightarrow{n \to \infty} W \iff \| W_n - W \|_\square \xrightarrow{n \to \infty} 0$$

In fact, the way to show that left & right convergence are equivalent is by showing that they are both equivalent to convergence in the cut metric.

For proofs, check the book "Large networks & convergent graph sequences" by Lovász (available online).
(For $\equiv$ w/ hom. density conv., check counting & inverse counting lemmas)

→ Relationship between the cut norm & L_p norms for graphons (and graphon distances) (codomain $[-1,1]$)

Let $W: [0,1]^2 \to [-1,1]$

Trivial inequalities: $\|W\|_\square \leq \|W\|_1 \leq \|W\|_2 \leq \|W\|_\infty \leq 1$

$\Rightarrow$ convergence in L_p, $p \geq 1$, implies cut norm convergence.

In the other direction, we have:

$$\|W\|_{2,2} \leq \sqrt{4\|W\|_{\infty\to 1}} \leq \sqrt{16\|W\|_\square}$$

$\Rightarrow$ convergence in cut norm implies convergence in L_2.

Pf.: We start by noting that

$$\|W\|_\square = \sup_{S,T \subseteq [0,1]} \left| \iint_{S\times T} W(u,v)\, du\, dv \right|$$

$$= \sup_{f,g : [0,1] \to [0,1]} \left| \int_0^1 \int_0^1 W(u,v) f(u) g(v)\, du\, dv \right|$$

$$\begin{cases} T_W f = \int_0^1 W(u,\cdot) f(u)\, du \\ (T_W f)(v) = \int_0^1 W(u,v) f(u)\, du \end{cases}$$

$$= \sup_{f,g : [0,1] \to [0,1]} \langle T_W f, g \rangle$$

Now, $\|W\|_{\infty\to 1}$ is defined as:

$$\|W\|_{\infty\to 1} = \sup_{-1 \le g \le 1} \|T_W g\|_1$$

$$= \sup_{-1 \le f,g \le 1} \langle T_W g, f \rangle$$

Rewriting this expression as :

$$\|W\|_{\infty \to 1} = \sup_{\substack{0 \leq f, f' \leq 1 \\ 0 \leq g, g' \leq 1}} \langle Tw(g - g'), f - f' \rangle$$

We get :

$$\|W\|_{\infty \to 1} \leq \sup_{0 \leq g, f \leq 1} \langle Twg, f \rangle$$

$$+ \sup_{0\,1 \leq g, f' \leq 1} \langle Twg, -f' \rangle$$

$$+ \sup_{0 \leq g', f' \leq 1} \langle -Twg', -f' \rangle$$

$$+ \sup_{0 \leq g', f' \leq 1} \langle -Twg', f \rangle$$

$$\leq 4 \|W\|_{\square}$$

For the first, use the Riesz-Thorin interpolation theorem for complex L_p spaces:

$$\|W\|_{p\to q} \leqslant \|W\|_{p_0\to q_0}^{1-\theta} \|W\|_{p_1\to q_1}^{\theta}$$

where $\theta = \min\left(1-\frac{1}{p}, \frac{1}{q}\right)$, $p_0, q_0 \in [1,\infty[$

w/ $\frac{1}{p} = \frac{1-\theta}{p_0}$ & $1-\frac{1}{q} = (1-\theta)\left(1-\frac{1}{q_0}\right)$,

and $p_1 = \infty$, $q_1 = 1$.

Define:

$$\cdot)\ \|W\|_{\square,\mathbb{C}} = \sup_{\substack{f,g:[0,1]\to\mathbb{C} \\ \|f\|_\infty, \|g\|_\infty \leq 1}} \left| \int_0^1\int_0^1 W(u,v) f(u) f(v)\, du\, dv \right|$$

For complex functions, we thus have:

$$\|W\|_{\infty \to 1} = \|W\|_{\square, \mathbb{C}} \leq 2 \|W\|_{\infty \to 1}$$

$\downarrow$ for complex functions

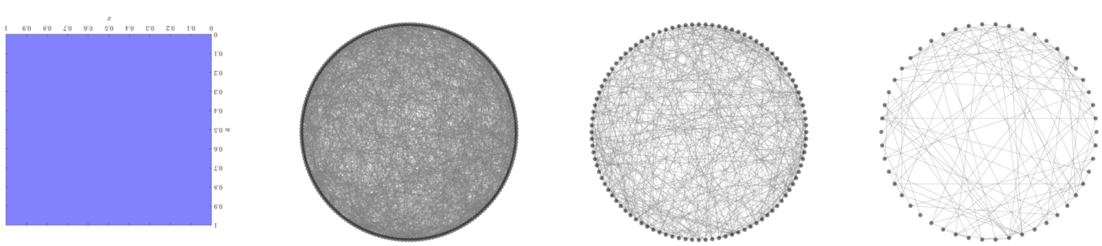
$\downarrow$ for real functions

Noting that $\|W\|_{p_0 \to q_0} \leq \|W\|_{1 \to \infty} \leq \|W\|_\infty \leq 1$ (since $W \leq 1$) completes the proof. ■

3) Can we use graphons to sample subgraphs?

Yes! They are generative models as well.

In fact, all of the graphs below were sampled from the graphon.



(a) 50 nodes (b) 100 nodes (c) 200 nodes (d) Graphon

How to sample?

•) "Template" graphs

The simplest way to sample a graph from W is by partitioning $[0,1]$ in a grid (regular partition):

$$I_1 \cup I_2 \cup \dots \cup I_n$$

where
$$I_j = \begin{cases} \left[\frac{j-1}{n}, \frac{j}{n}\right[, & 1 \leq j \leq n-1 \\ \left[\frac{n-1}{n}, 1\right] , & j = n \end{cases}$$

and the node labels are $u_j = \frac{j-1}{n} \quad \forall j$

We then define the template graph G_n via its adjacency,

$$[A_n]_{ij} = W(u_i, u_j)$$

i.e., it is a weighted graph.

•) Random weighted graphs

Another type of graph we can sample from W are graphs with random nodes, where the u_j are sampled randomly from $[0,1]$, typically, uniformly, i.e.:

$$u_j \sim \text{Uniform}[0,1]$$

The edges are then defined in the same way as for template graphs:

$$[A_n]_{ij} = W(u_i, u_j)$$

i.e., it is a weighted graph

•) "Fully" random graphs (a.k.a. W-random graphs)

These are graphs with both random nodes & edges. The node labels are once again sampled as:

$$u_j \sim \text{Uniform}([0,1])$$

and the edges as:

$$[A_n]_{ij} \sim \text{Bernoulli}(W(u_i, u_j))$$

The edges are unweighted and undirected.

All of the graphs above converge to W in some sense

- Template: trivial. Convergence in L_2 implies $\|\cdot\|_\square$ convergence (deterministic)
- Weighted: sampling lemma ①:

w.p. at least $1 - \exp\left(\frac{-n}{2\log n}\right)$,

$$\delta_\square(G_n, W) \leq 20/\sqrt{\log n}$$

- Random: sampling lemma ②:

w.p. at least $1 - \exp\left(\frac{-n}{2\log n}\right)$,

$$\delta_\square(G_n, W) \leq 22/\sqrt{\log n}$$

in probability

We'll look at the proof later.

d) GNN continuity, i.e., GNN convergence?

This question has a long answer.

To start to answer it, we need to introduce graphon signals

▶ Graphon Signal processing

A graphon signal is defined as a function

$\mathcal{X} : [0,1] \to \mathbb{R} \qquad (x \in \mathbb{R}^n)$

We focus on signals in L_2, $\mathcal{X} \in L_2([0,1])$:

$$\int_0^1 |\mathcal{X}(u)|^2 du \leq B < +\infty$$

"Finite energy signals"

Like a graphon, graphon signals are limits of convergent sequences of graph signals

Induced graphon signals: Let (G_n, x_n) be a graph signal. The induced graphon signal is defined as:

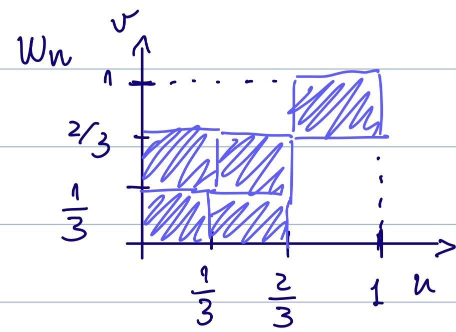
W_n is as in $(*)$

$$\mathfrak{X}_n(u) = \sum_{j=1}^{n} [x_n]_j \, \mathbb{I}(u \in I_j)$$

$\mathbb{I}$ is indicator fcn; $I_j = \begin{cases} \left[\frac{j-1}{n}, \frac{j}{n}\right), & 1 \leq j \leq n-1 \\ \left[\frac{n-1}{n}, 1\right], & j = n \end{cases}$

E.g.:

$$A_n = \begin{array}{c|ccc|c} & 1 & 2 & 3 & \\ \hline 1 & 1 & 1 & 0 & 3 \\ 2 & 1 & 1 & 0 & 2 \\ 3 & 0 & 0 & 1 & 1 \\ \hline \end{array}$$



$$x_n = \begin{array}{|c|c} 0.5 & 1 \\ 1 & 2 \\ 0.5 & 3 \end{array}$$