Graphon Mixtures

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CSIRO's Data61

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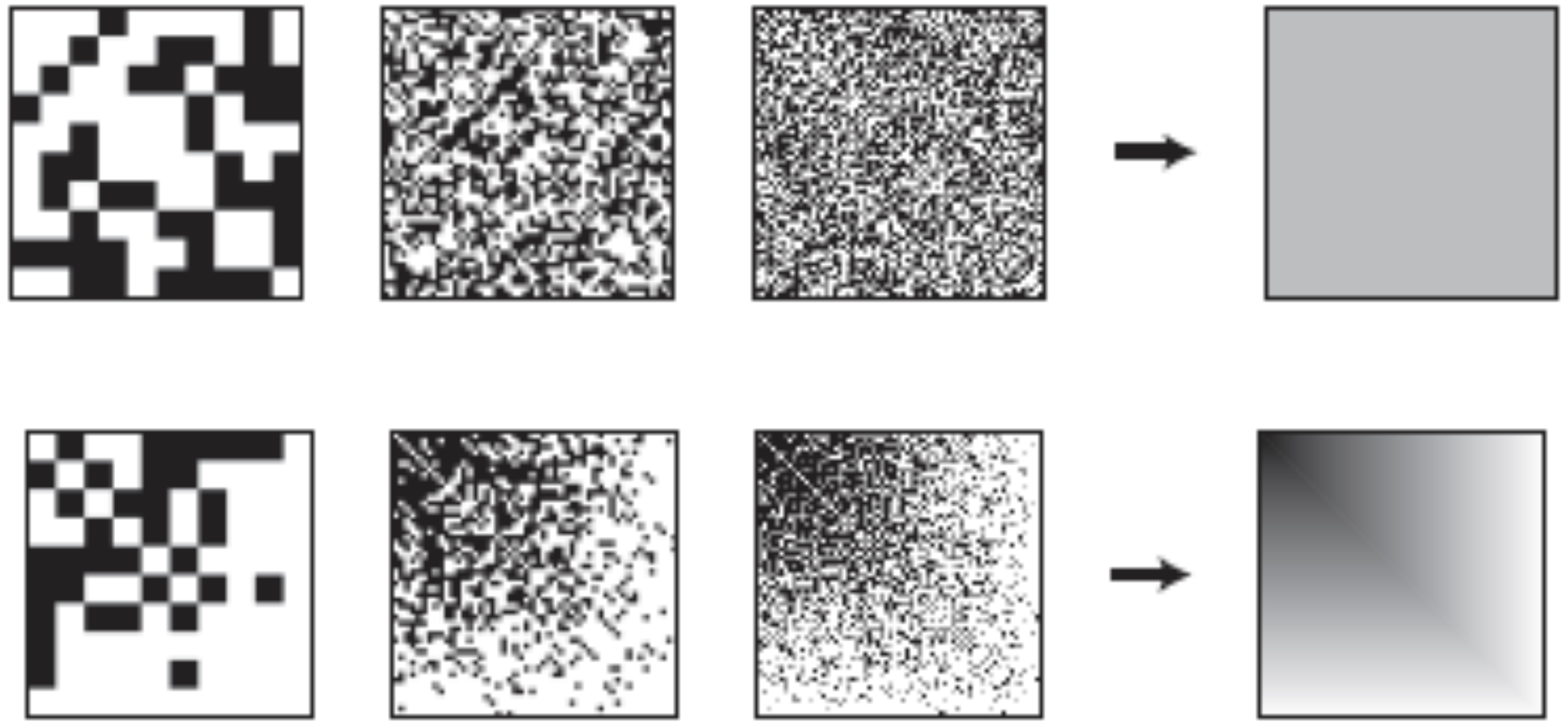
Graphons

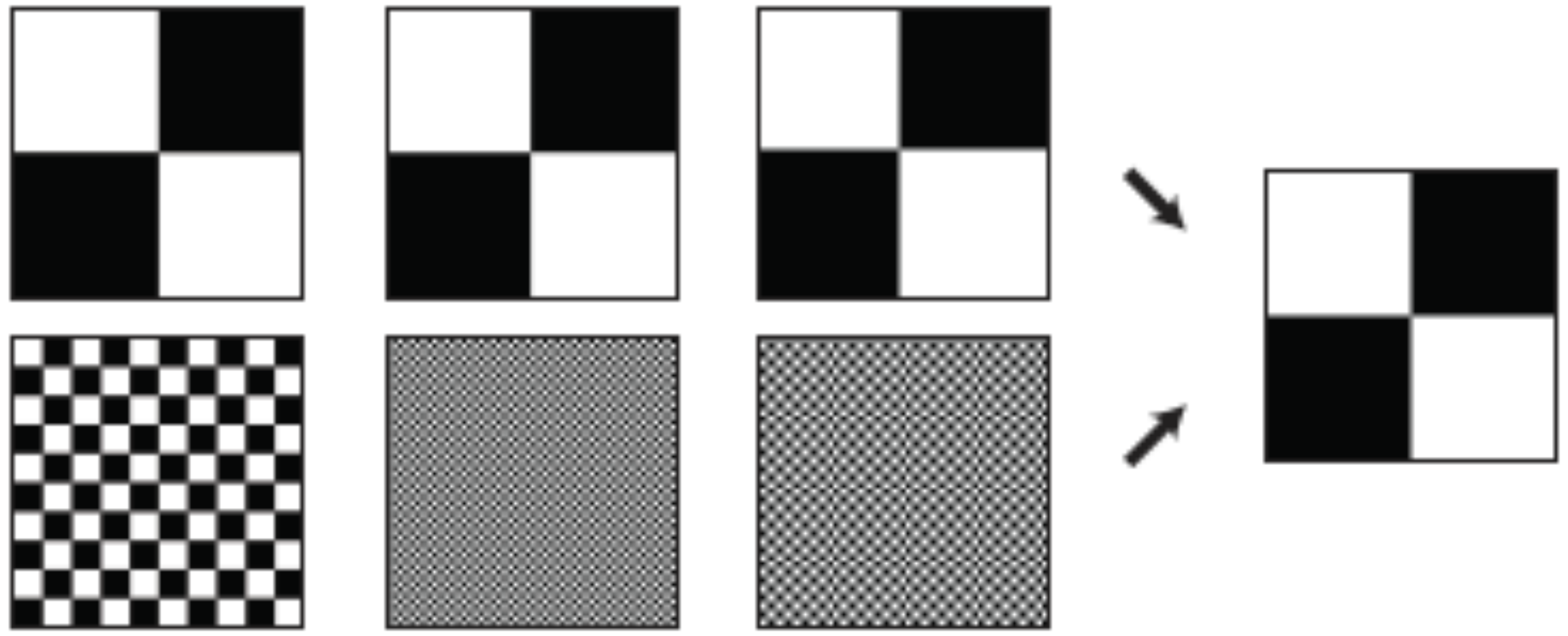
What are graphons?

- Graph limits $W : [0,1]^2 \to [0,1]$
- Map the adjacency matrix to the unit square (empirical graphons) and take a limit

Erdos-Renyi graphs



Growing uniform attachment graphs

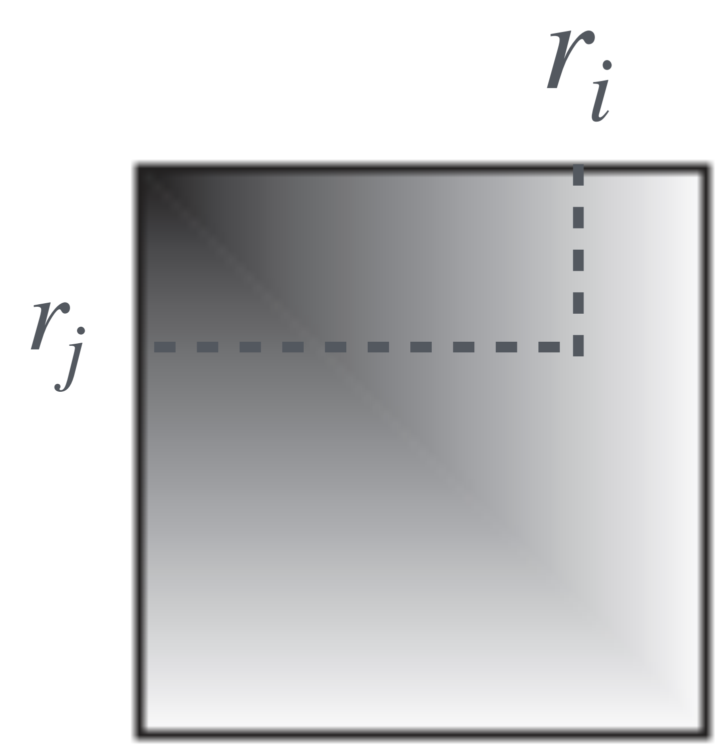


Bi-partite graphs

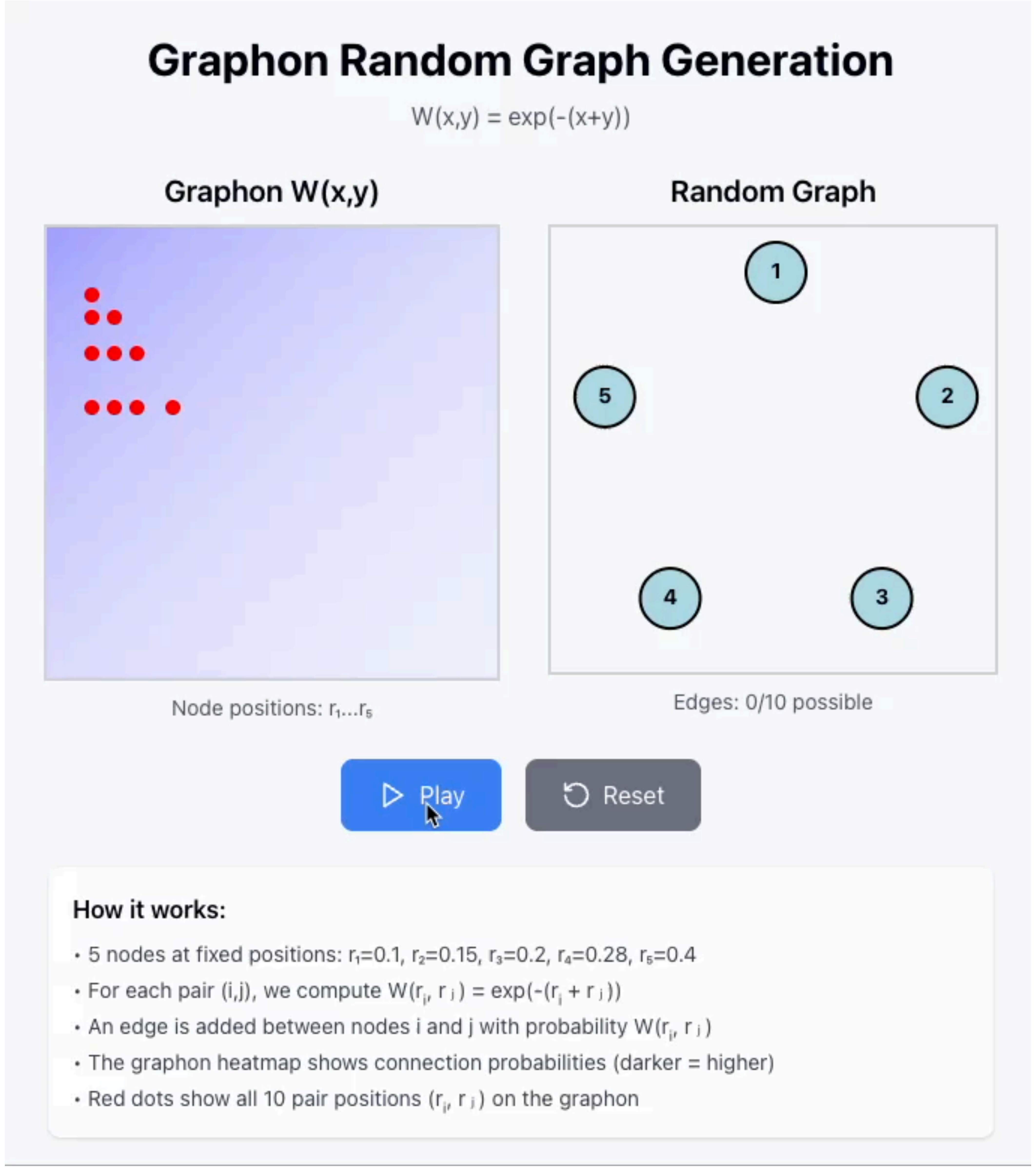
Glasscock, D. (2015). What is... a graphon. *Notices of the AMS*, *62*(1), 46-48.

How can we use graphons?

- To generate new graphs (sample graphs)
- Sampling - a graph with n nodes labeled $\{1,2,\ldots,n\}$
  - Sample n random points from the interval $[0,1]$ - $\{r_1, r_2, \ldots, r_n\}$
  - For every (r_i, r_j) the value $W(r_i, r_j) = p$ is the edge probability
  - Toss a coin with probability p, and connect the edge between i and j if you get heads

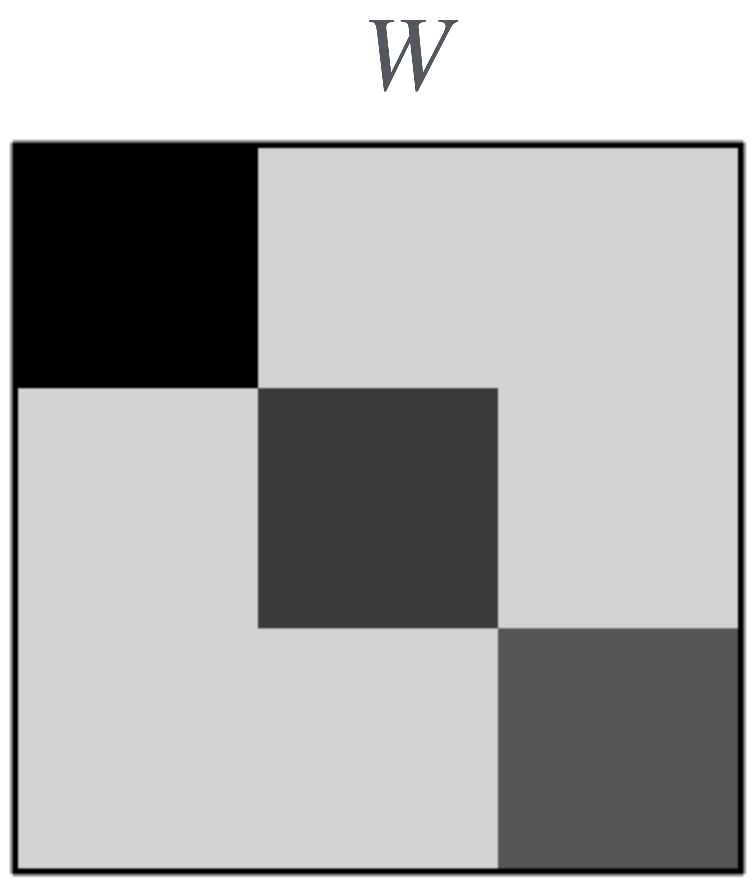


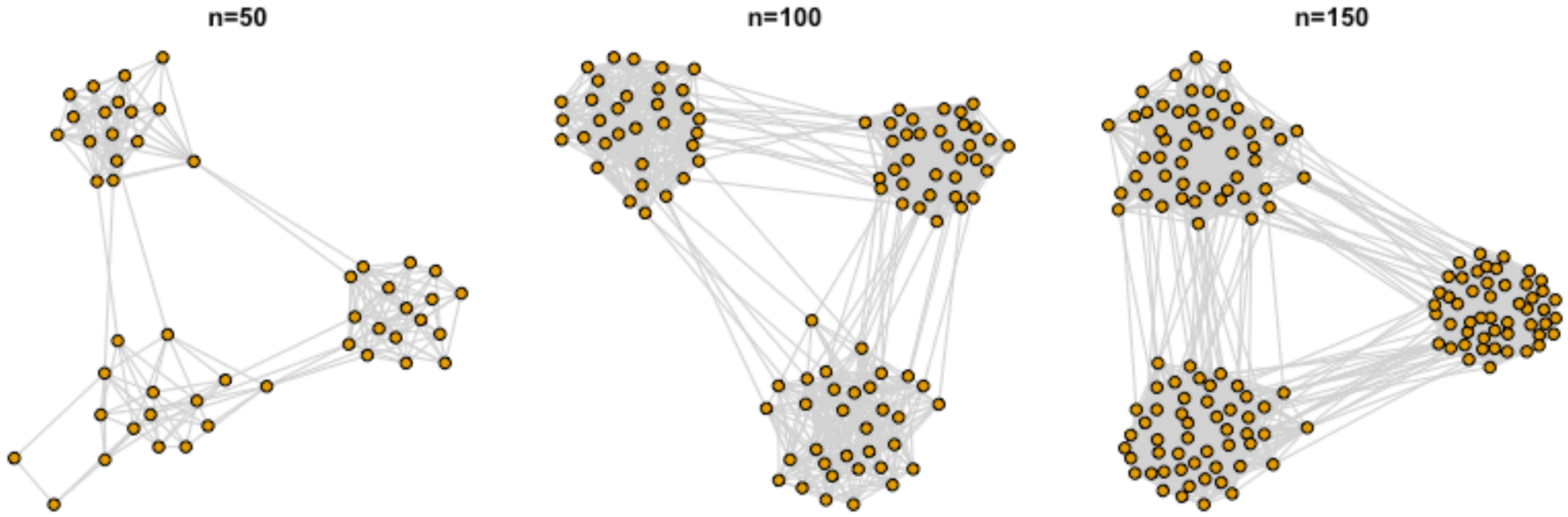
Animation made using Claude



https://claude.ai/public/artifacts/67f1ef89-fef2-4634-8812-f35b6350653e

Graphons as graph generators

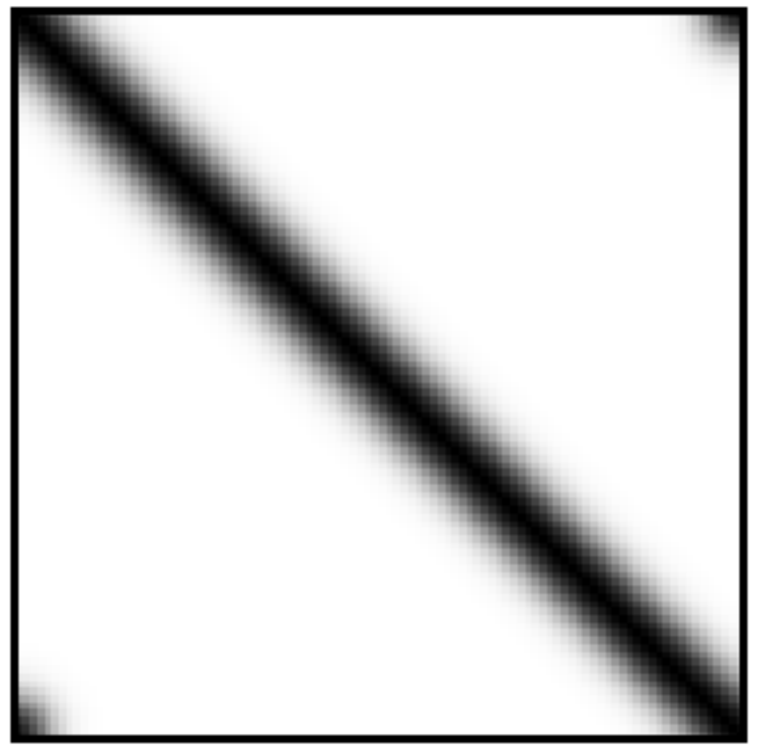


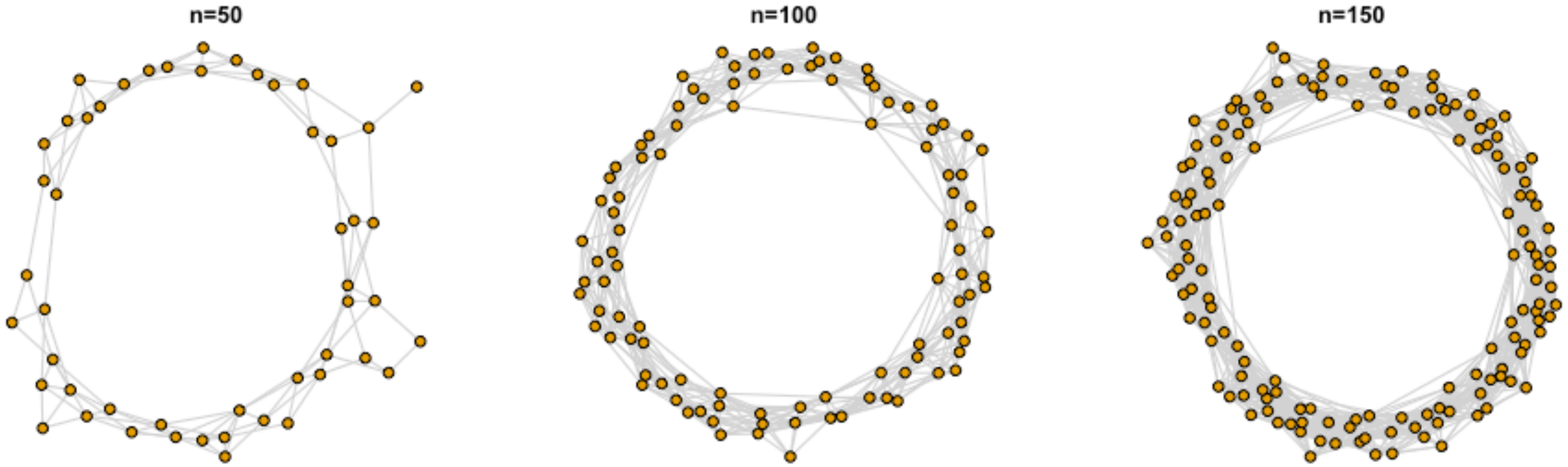


- Classical Stochastic Block Model type graphon

Graphons as graph generators

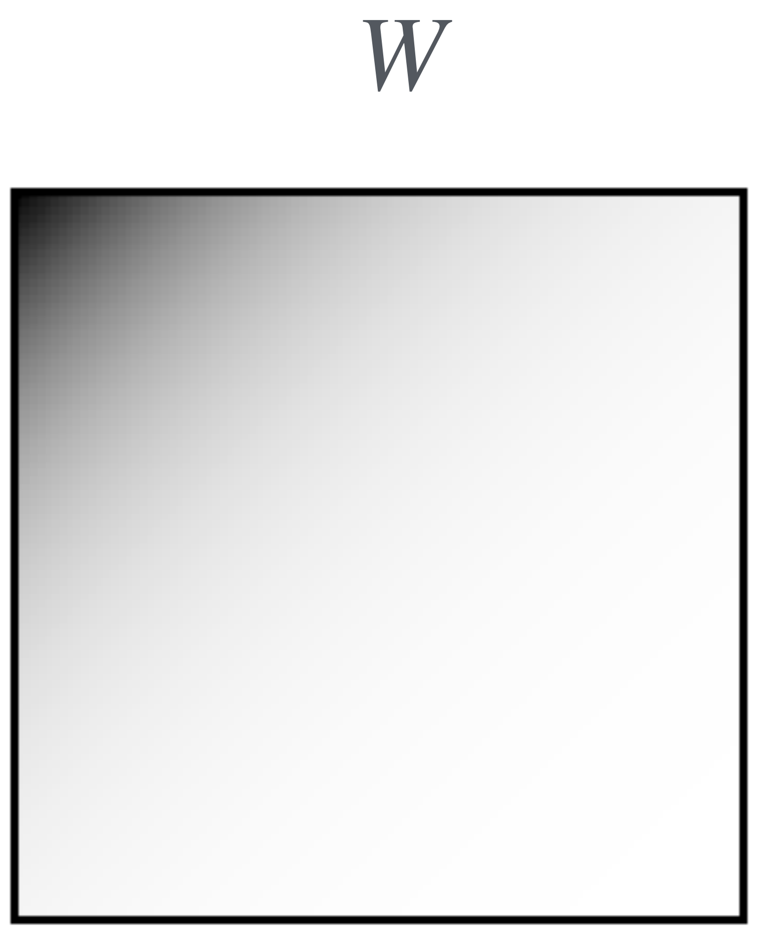
W

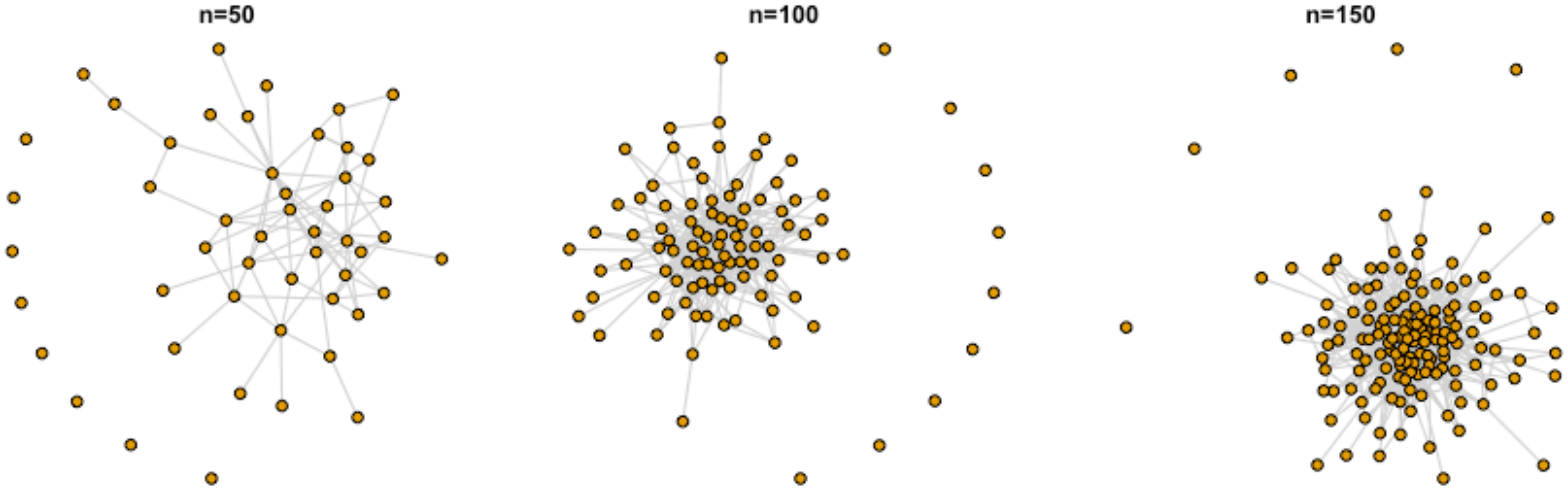




- Graph generated from W has a ring structure (but dense)

Graphons as graph generators

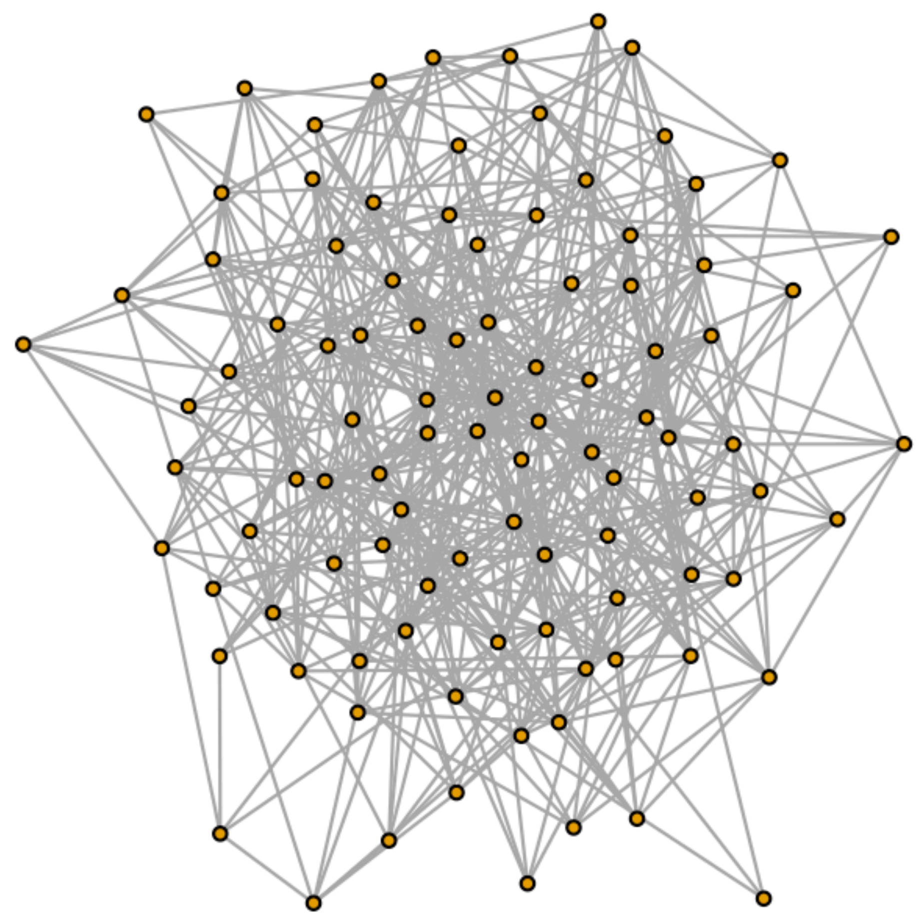




- $W = \exp(-(x+y)/30)$

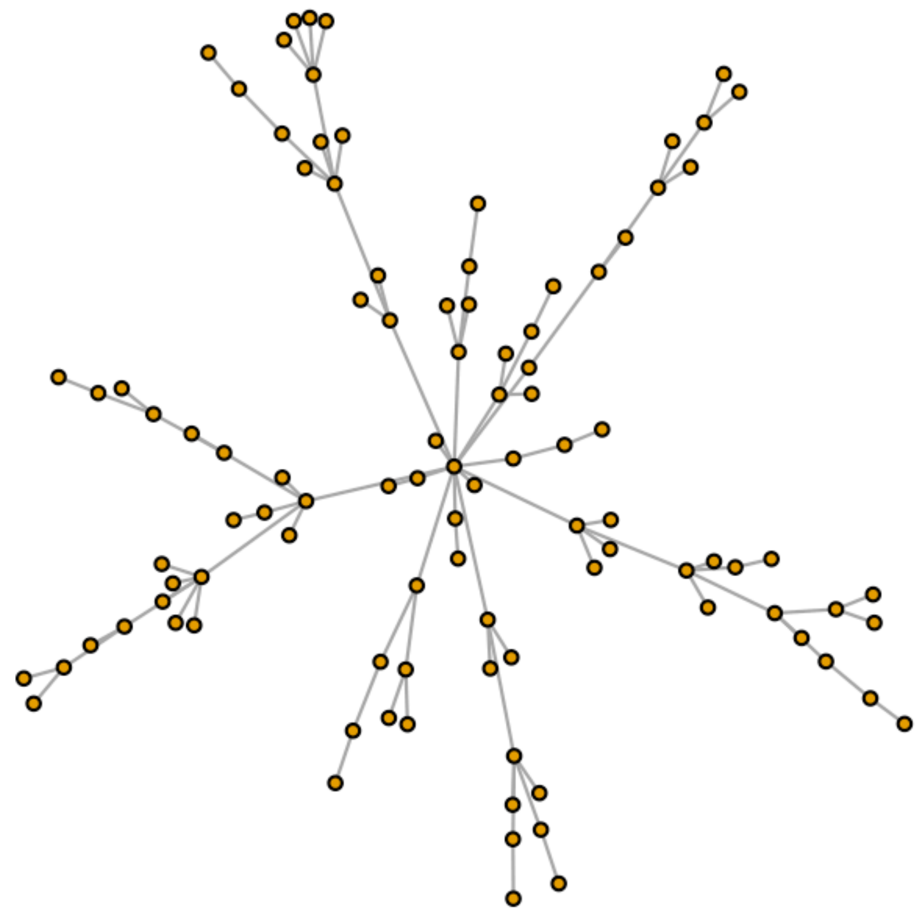
Dense and sparse graphs

Dense



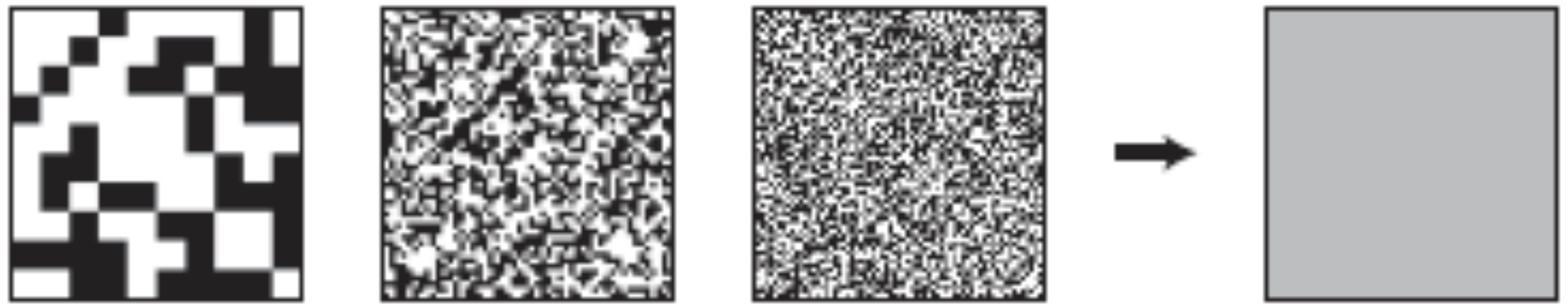
- Consider a graph sequence $\{G_n\}_n$, where G_n has n nodes and m edge
- Dense graphs: $\liminf_{n\to\infty} \frac{m}{n^2} = c > 0$
  - **Edges grow quadratically with nodes**
- Sparse graphs: $\lim_{n\to\infty} \frac{m}{n^2} = 0$
  - **Edges grow subquadratically with nodes**

Sparse



Limitation of traditional graphons

- ***Graphs represented by a graphon are either trivially empty or dense***
- These graphons can model dense graphs but not sparse graphs



- Why?
  - The volume from $(x, y, W(x, y))$ converges to $\lim_{n\to\infty} \frac{2m}{n^2}$
  - For sparse graphs $\lim_{n\to\infty} \frac{m}{n^2} = 0 \iff W = 0$

What happens when $W = 0$?

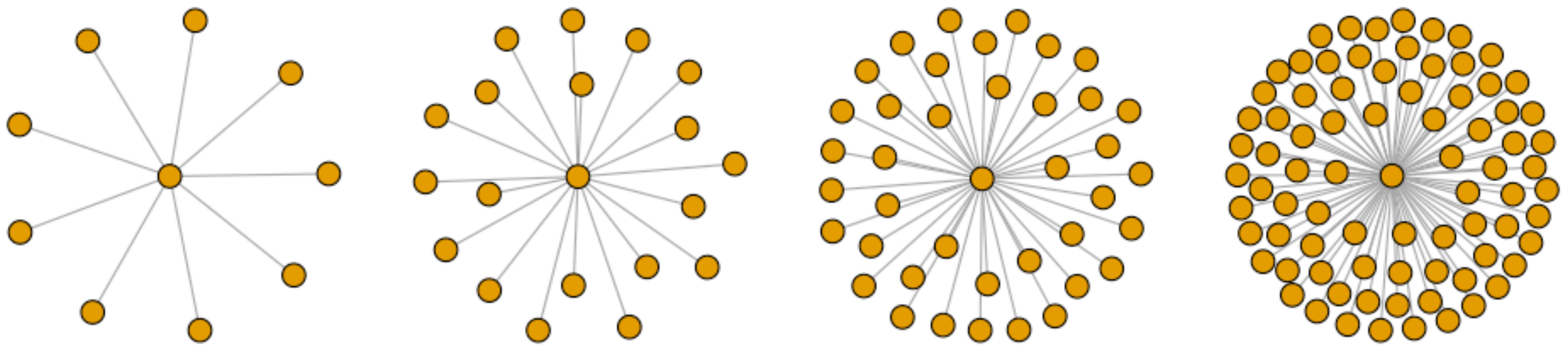
$W = 0$

- Sample n random points from the interval $[0,1]$ - $\{r_1, r_2, \ldots, r_n\}$
- For every (r_i, r_j) the value $W(r_i, r_j) = 0$ is the edge probability
- You have a graph with n nodes, but no edges — not representative of sparse graphs

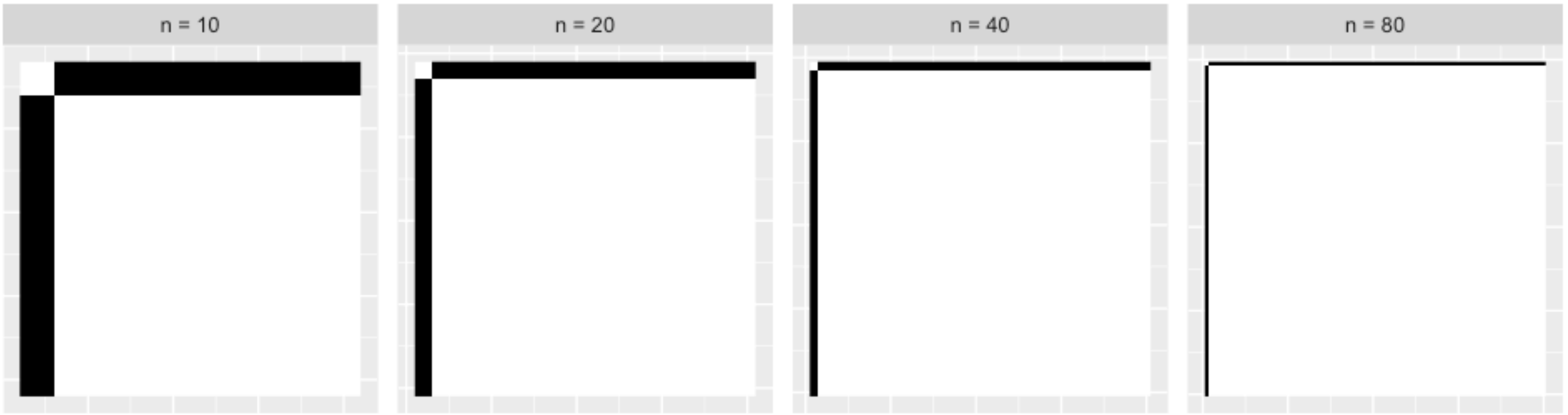
This is the fundamental problem of modeling sparse graphs using graphons!

Example - Star graphs $K_{1,n}$

- Star graphs

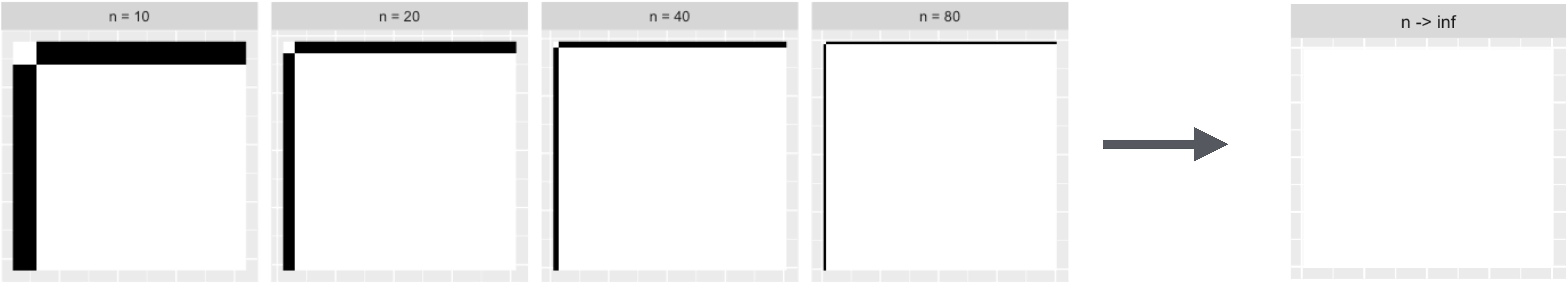


- Adjacency matrix pixel pictures
  ones - black
  zeros - white



For sparse graphs …

- Pixel pictures (empirical graphons) converge to zero



Empirical graphons

Graphon

What about other non-graphon methods?

- Yes, other generative methods exist
  - Eg. Preferential attachment graphs
- But graphons are non-parametric, very flexible
  - Modeling the full adjacency matrix
  - Interest in pursing graphons for sparse graphs

Current approaches - graphons + sparse graphs

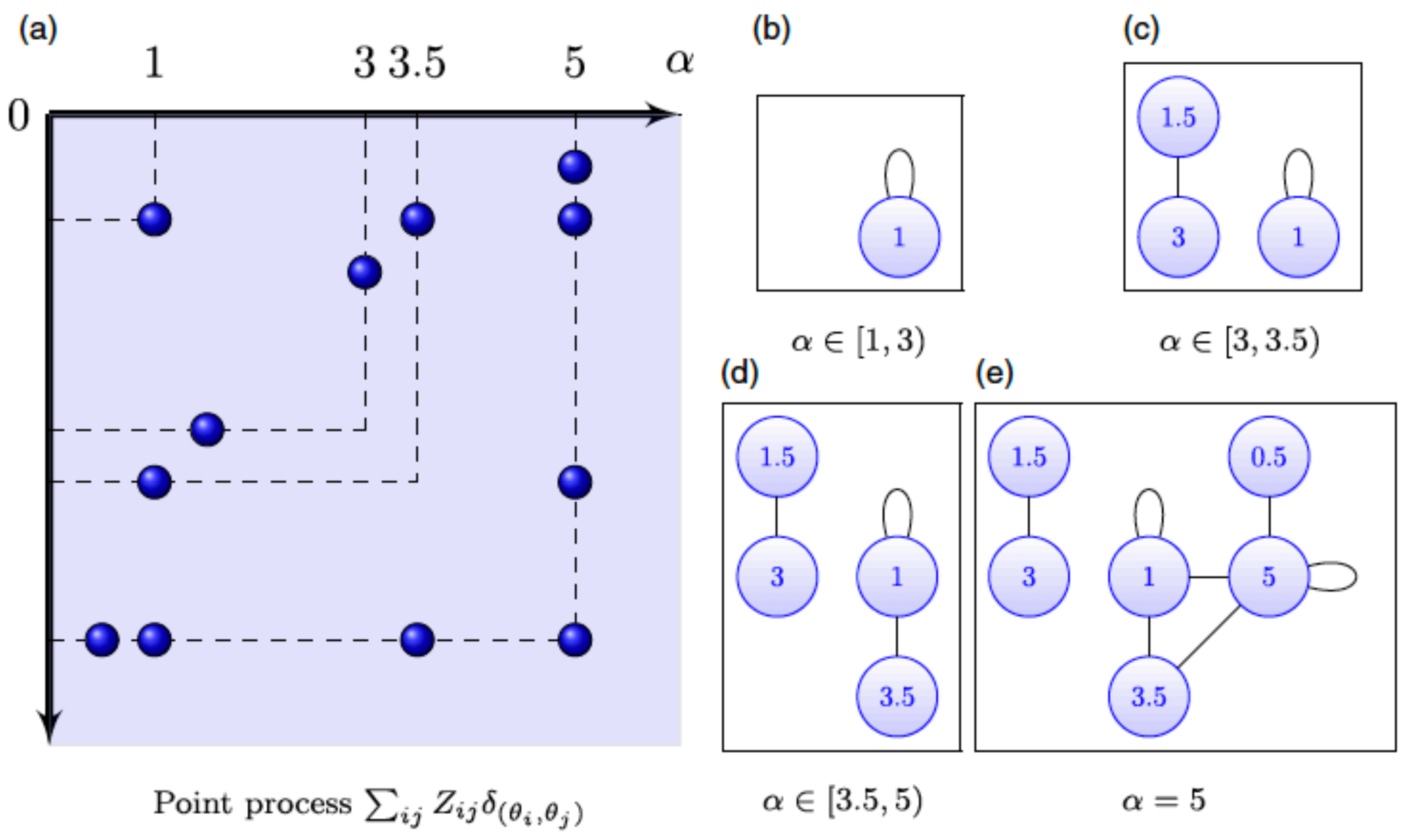
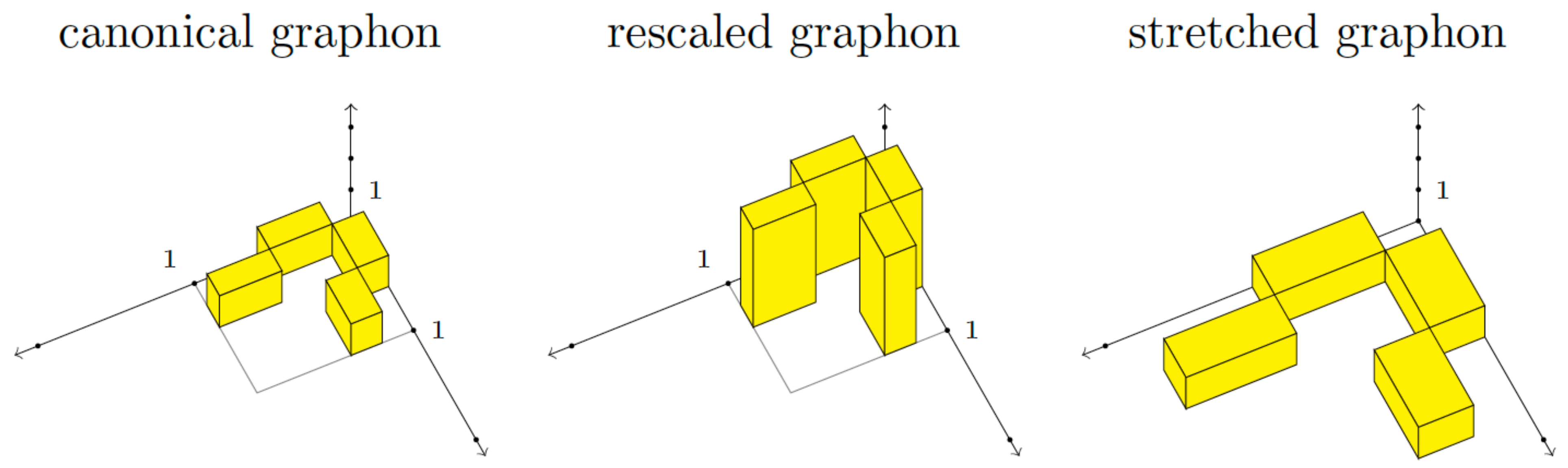


FIGURE 3. Illustration of the connection between the point process on the plane and the graphex process. (a) Point process $\sum_{ij} Z_{ij}\delta_{(\theta_i,\theta_j)}$ on the plane. (b–e) Associated graphs $\mathcal{G}_\alpha$ for (b) $\alpha \in [1, 3)$, (c) $\alpha \in [3, 3.5)$, (d) $\alpha \in [3.5, 5)$, and (e) $\alpha = 5$. Note that the graph is empty for $\alpha < 1$.



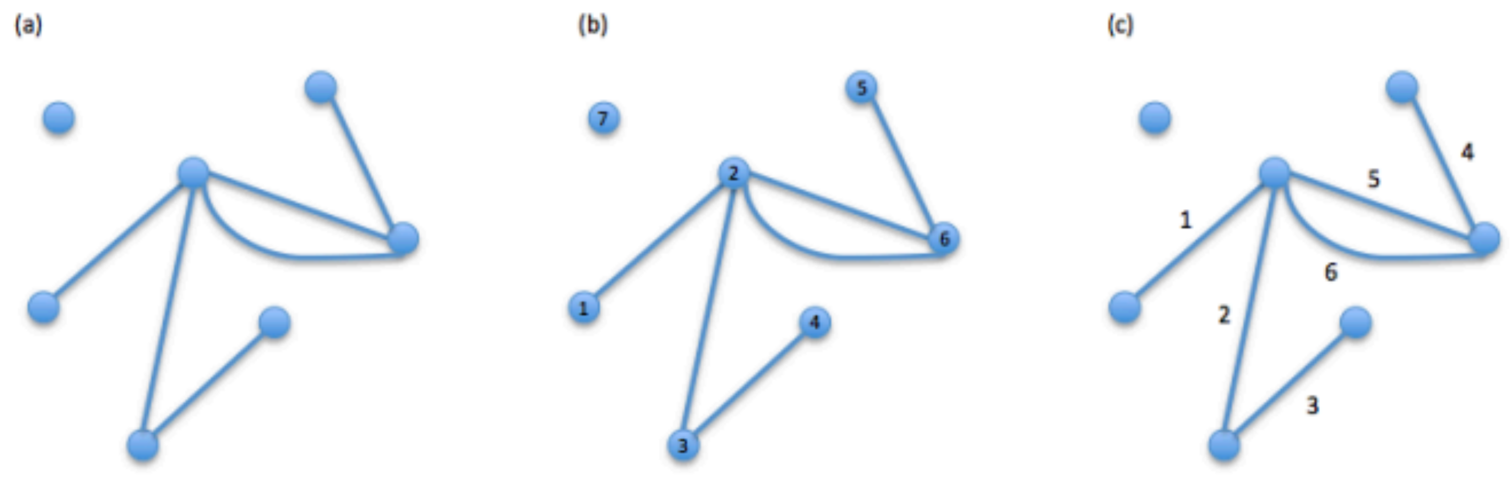


FIGURE 1. (a) A network structure derived from some process of interactions. Neither vertices nor edges come equipped with labels. (b) Network obtained by labeling vertices of network in Panel (a). (c) Network obtained by labeling edges of network in Panel (a).

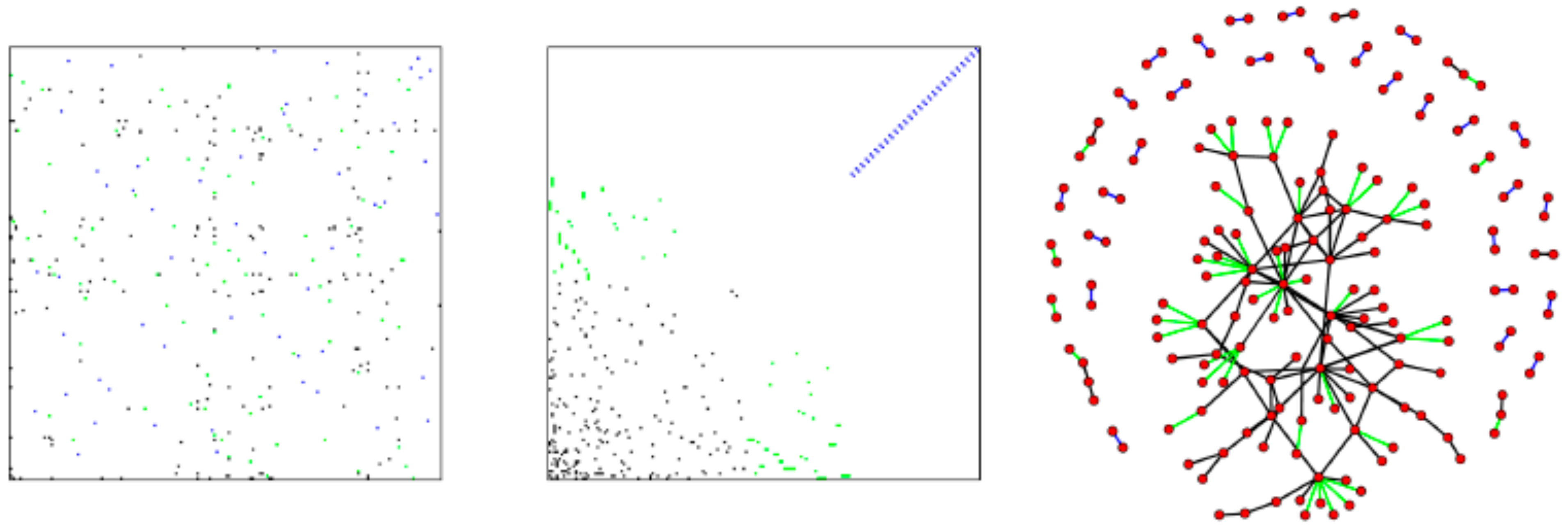


FIGURE 3. Realization of unlabeled graphex process generated by $\mathcal{W} = (I, S, W)$ at size $s = 15$ (right panel), and associated dilated empirical graphon (left and center panels). The generating graphex is $W = (x+1)^{-2}(y+1)^{-2}$, $S = 1/2\exp(-(x+1))$, and $I = 0.1$. The observation size is $s = 15$. The dilated empirical graphex is

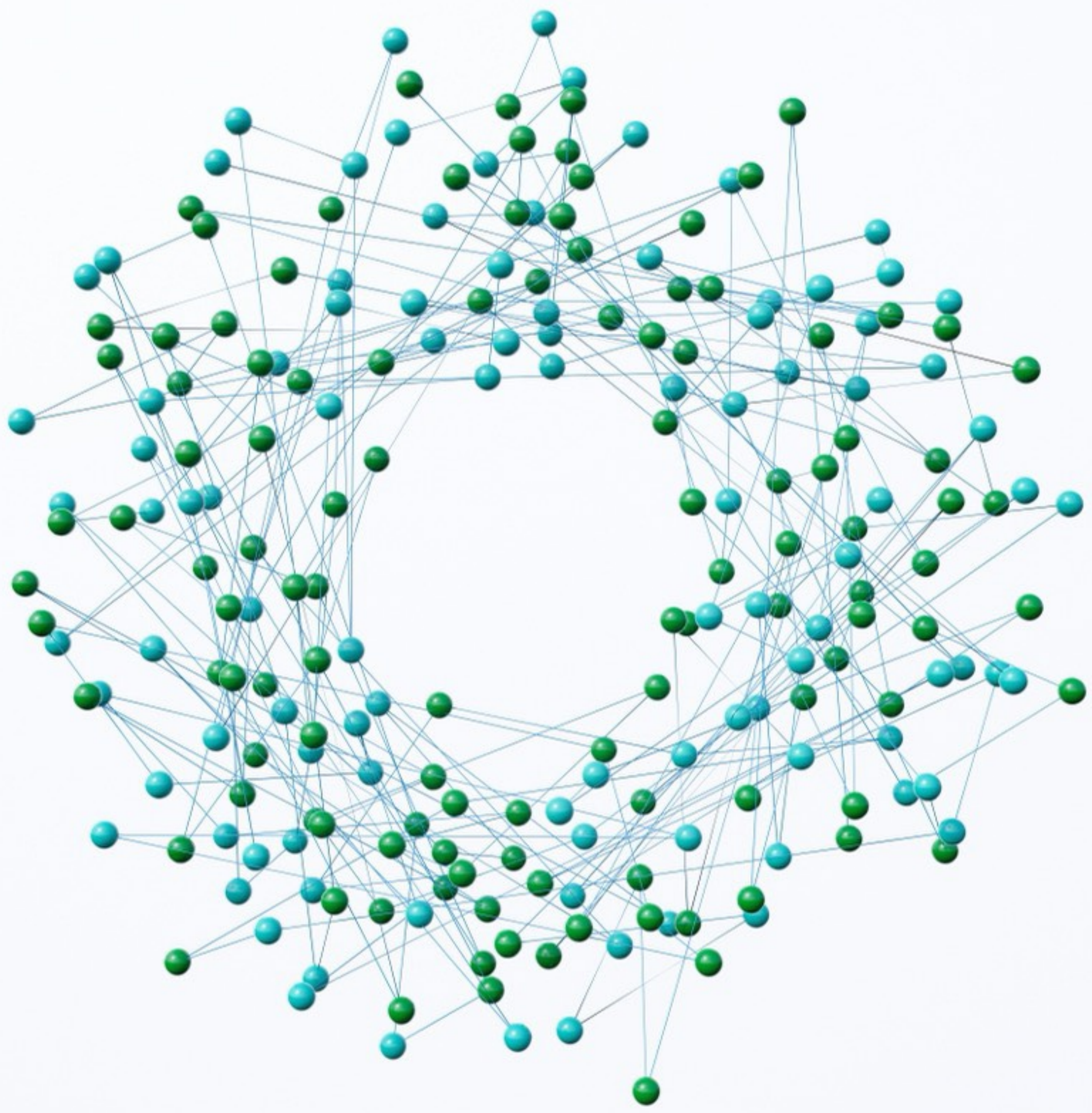
Caron, F., & Fox, E. B. (2017). Sparse graphs using exchangeable random measures. Journal of the Royal Statistical Society Series B: Statistical Methodology, 79(5), 1295-1366.

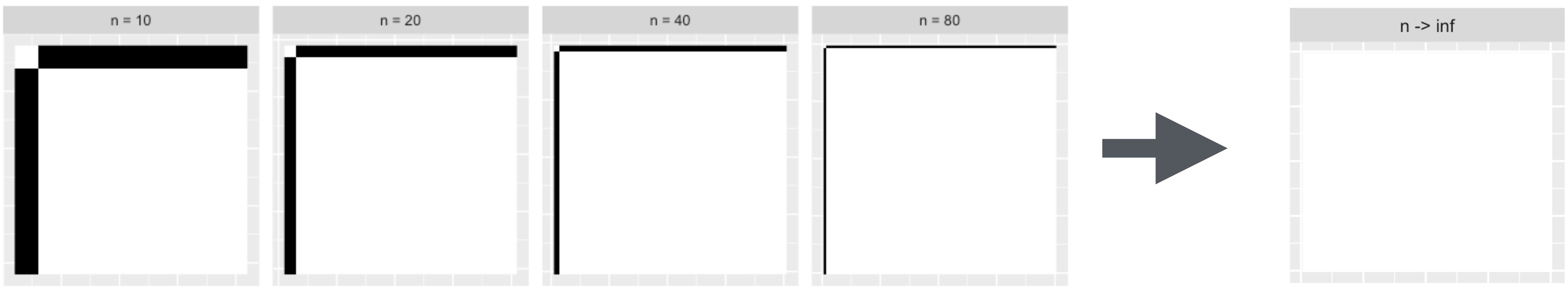
Borgs, C., Chayes, J. T., Cohn, H., & Holden, N. (2018). Sparse exchangeable graphs and their limits via graphon processes. Journal of Machine Learning Research, 18(210), 1-71.

Crane, H., & Dempsey, W. (2016). Edge exchangeable models for network data. arXiv preprint arXiv:1603.04571.

Veitch, V., & Roy, D. M. (2015). The class of random graphs arising from exchangeable random measures. *arXiv preprint arXiv:1512.03099*.

Proposed method





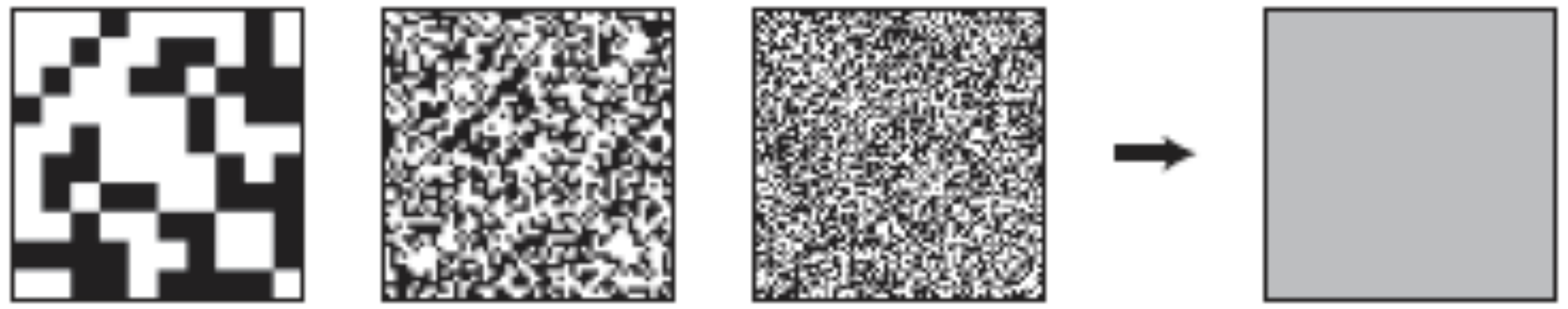
$\{G_n\}_n$

Transform $\{G_n\}_n$ such that

Model $\{G_n\}_n$ as it is

— the transformed graphs are dense

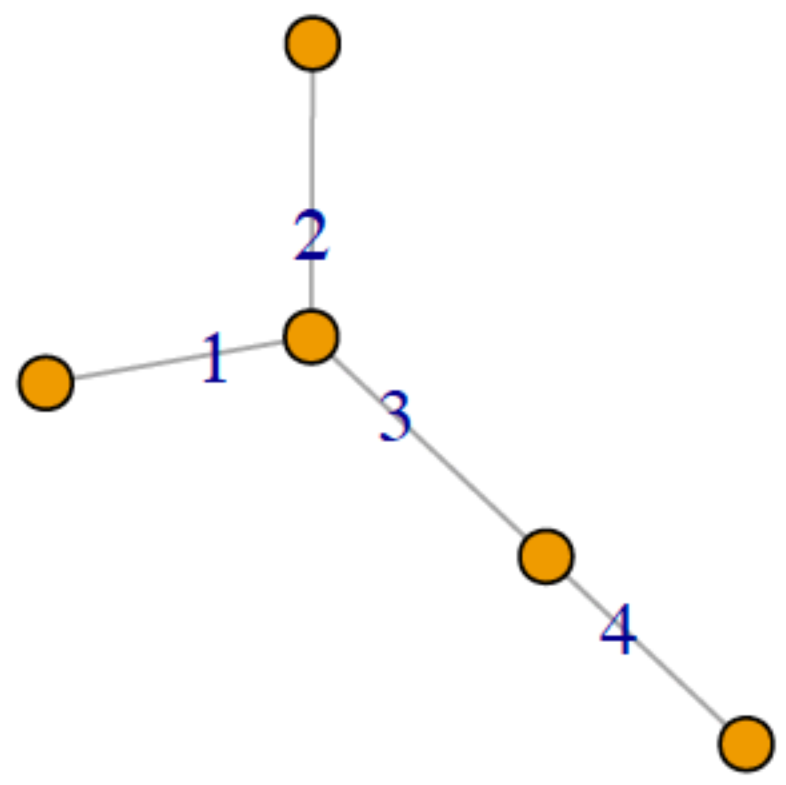
— Complex mathematical approaches



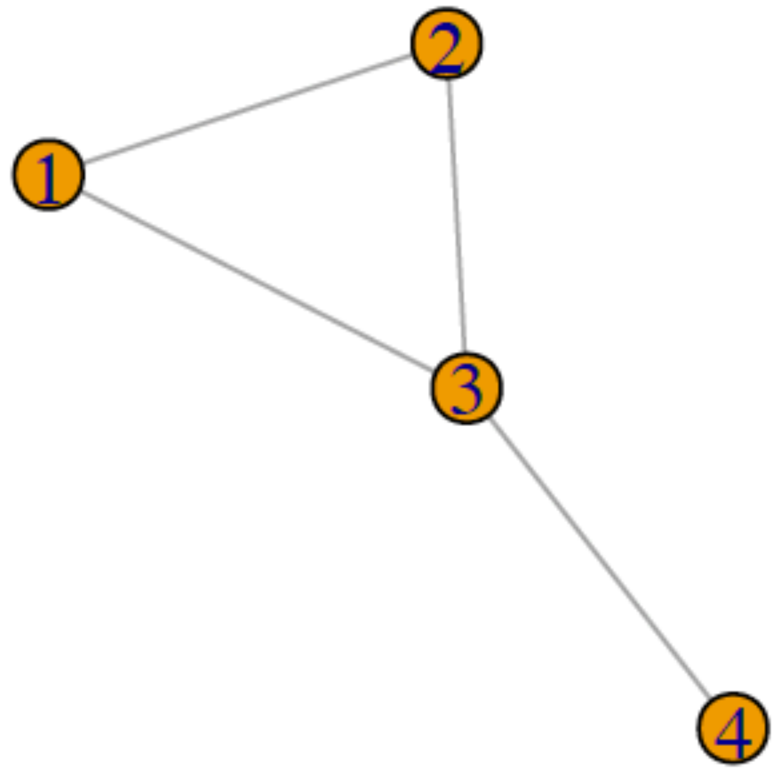
— Works for a subset of sparse graphs

The transformation - line graphs

- Edges Mapped to vertices
- Vertices are connected, if they share an edge
- Work originated by Hassler Whitney in 1932



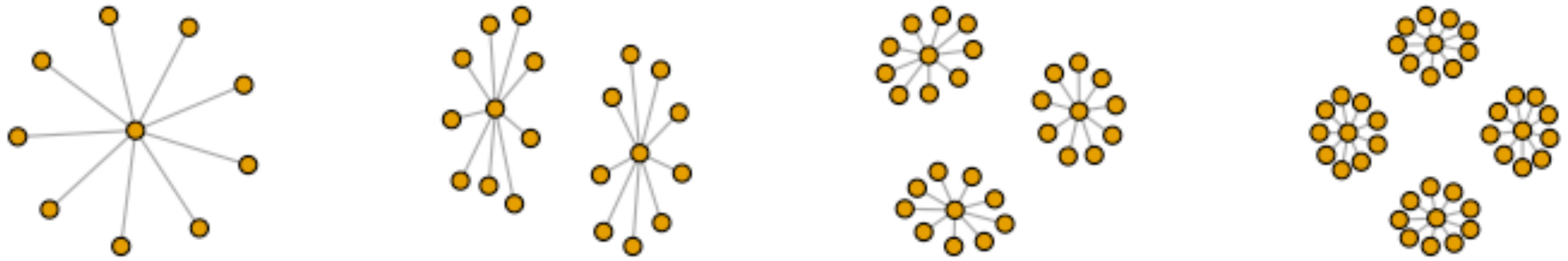
Graph G



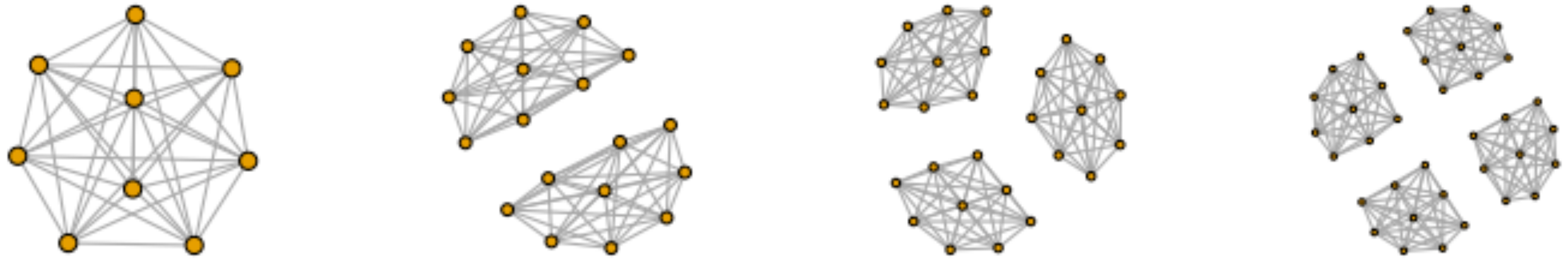
Line graph $H = L(G)$

Star graphs

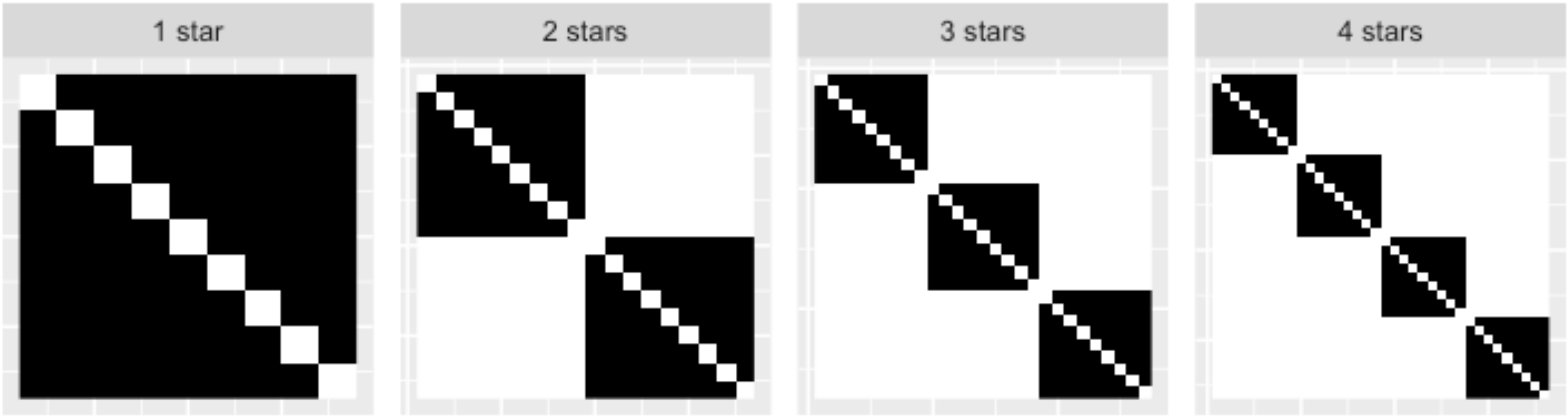
- Star graphs G_n



- Line graphs of stars (complete subgraphs)
  $H_m = L(G_n)$



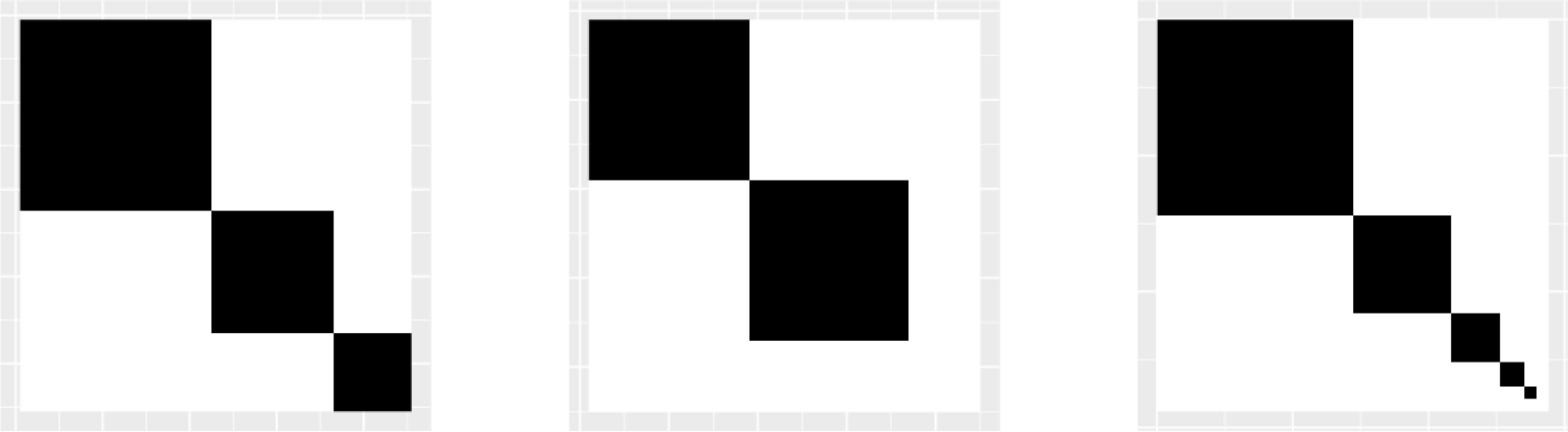
- Empirical graphons of line graphs



Kandanaarachchi, S., & Ong, C. S. (2024). Graphons of line graphs. *arXiv preprint arXiv:2409.01656*.

Line graph limits

- ***Janson (2016): A graph limit is a line graph limit if and only if it is a disjoint clique graph limit***.

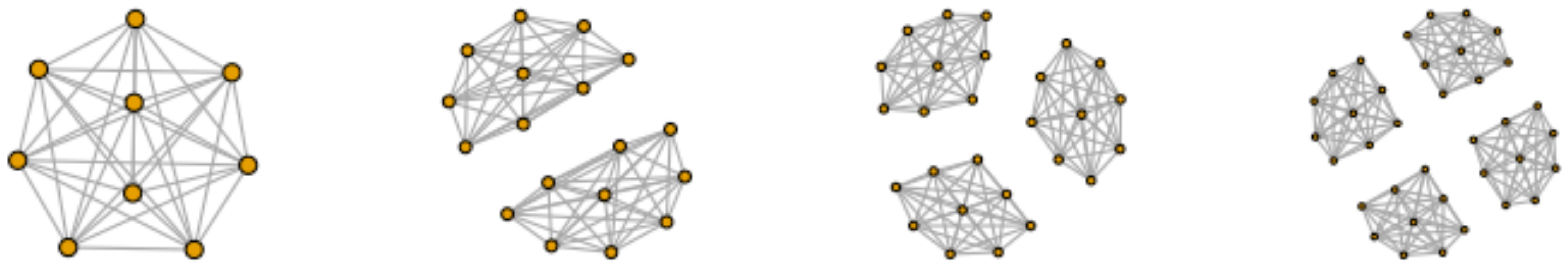


Examples of line graph graphons

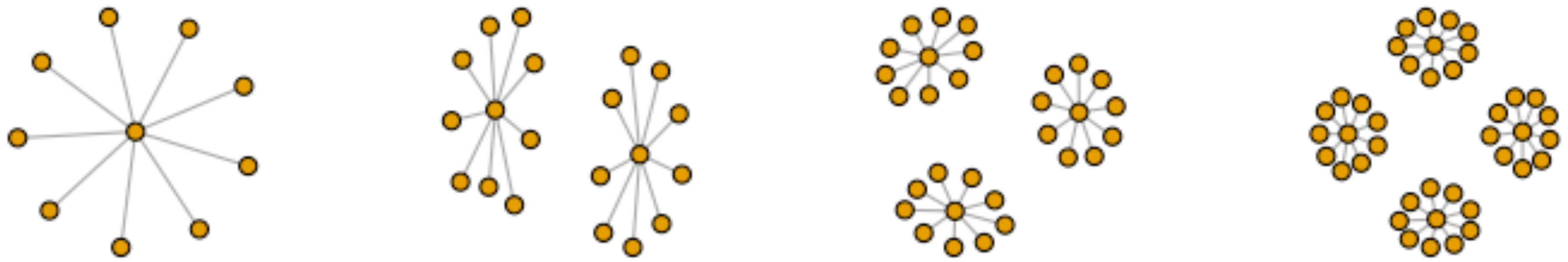
Janson, S. (2016). Graph limits and hereditary properties. *European Journal of Combinatorics*, *52*, 321-337.

Graphs sampled from line graph limits

- They are disjoint cliques



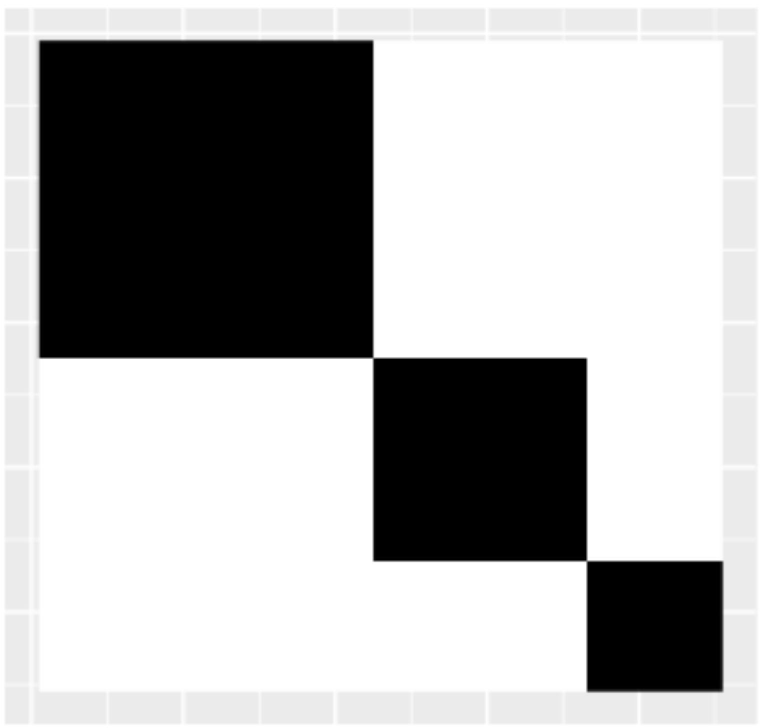
- The inverse line graphs of disjoint cliques are stars

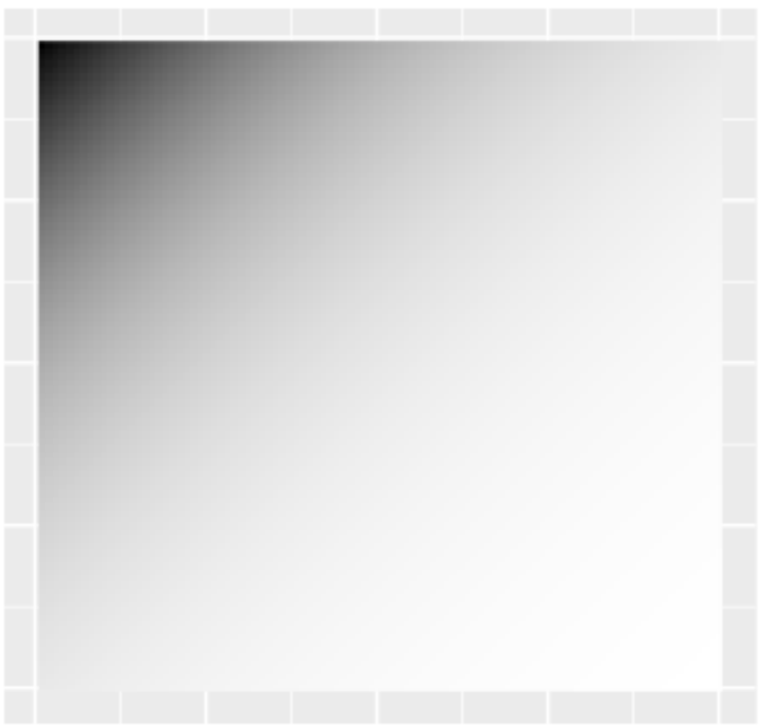


- ***The inverse line graph exists when you sample from a line graph limit; and they are disjoint stars.***

Graphon Mixtures

(U, W) graphon mixture

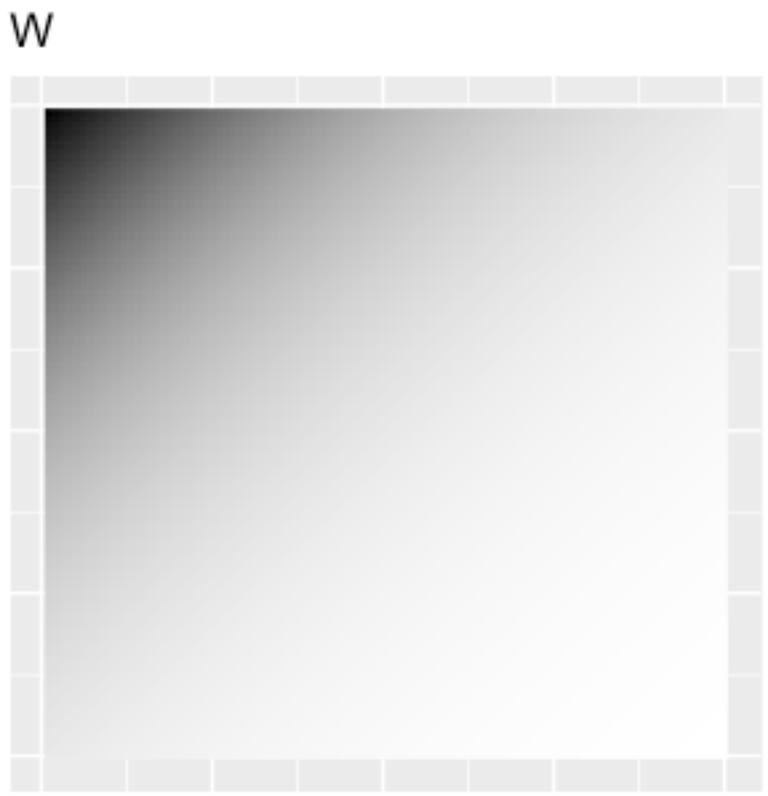


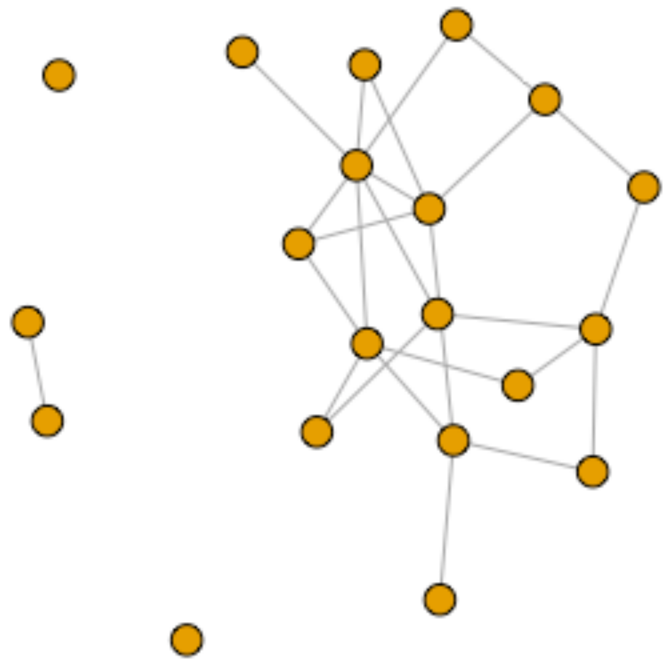


- U is a disjoint clique graphon, W is a graphon
- $\{n_{d_i}\}_i$ and $\{m_{s_i}\}_i$ are increasing positive integer valued sequences
- G_{d_i} - graph sampled from W with n_{d_i} nodes
- H_{s_i} - graph sampled from U with m_{s_i} nodes => $G_{s_i} = L^{-1}(H_{s_i})$ is a collection of stars
- New edges for joining $m_{new_i} = cm_{d_i}$ for some small c
- Join G_{d_i} (the dense part) with G_{s_i} (the sparse part) with m_{new_i} edges
- Call the joined graph G_{n_i}. We get a mixture graph sequence $\{G_{n_i}\}_i$

Kandanaarachchi, S., & Ong, C. S. Graphon Mixtures. *AISTATS 2026*.

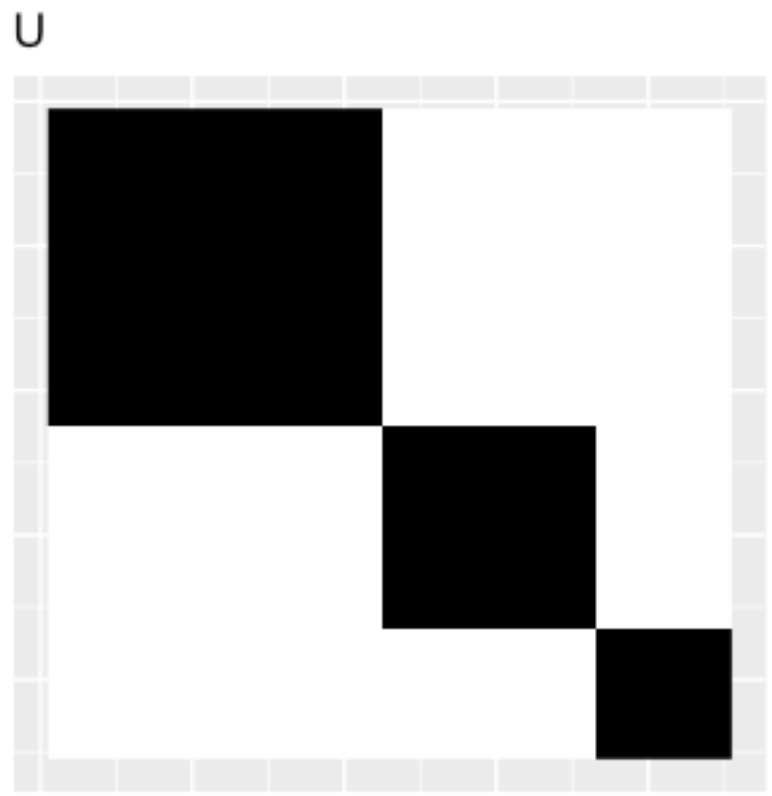
Graphon mixtures





Sample dense graph

G_{n_d}

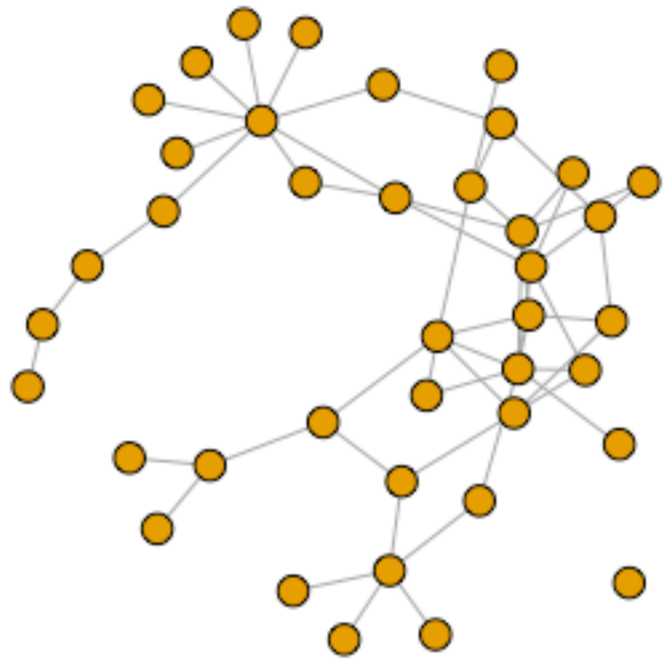


Sample sparse graph

$G_{n_s} = L^{-1}(H_{m_s})$

First sample disjoint cliques
Then compute the inverse line graph

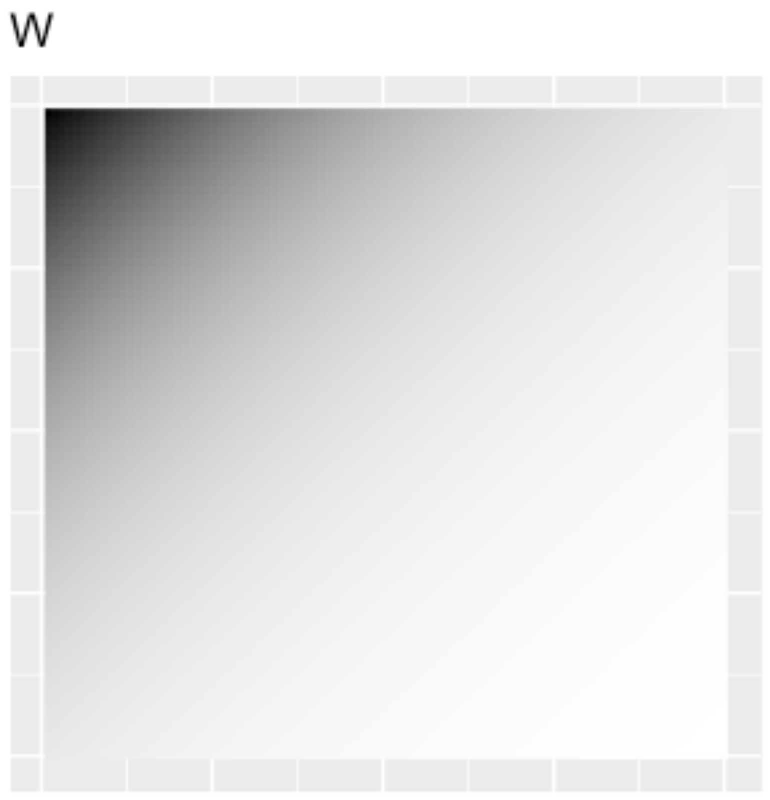
Randomly join the two graphs

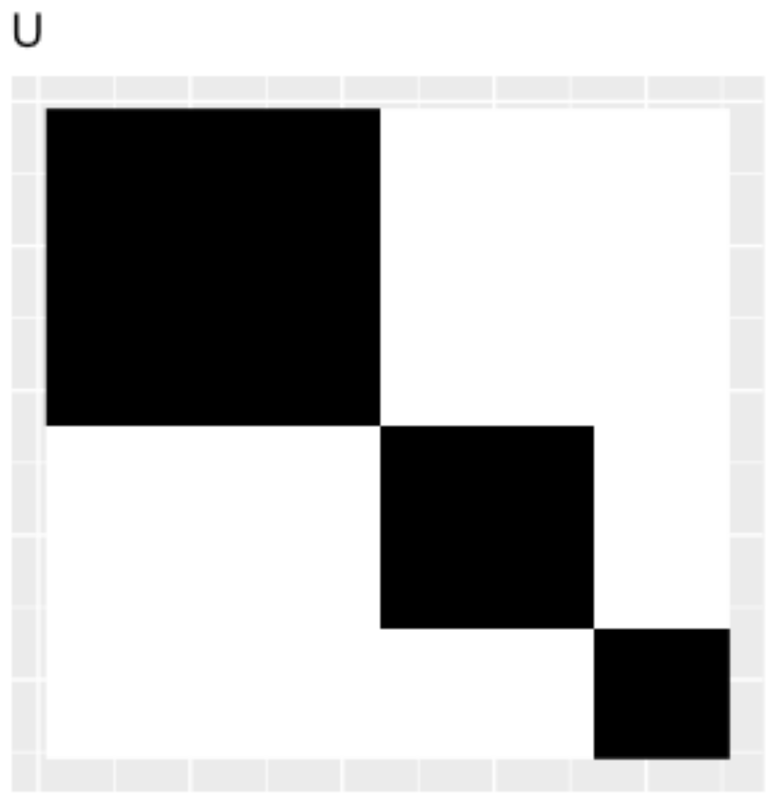


- Parameters: dense nodes n_d, sparse edges m_s, the number of edges when joining m_{new}

Kandanaarachchi, S., & Ong, C. S. Graphon Mixtures. *AISTATS 2026*.

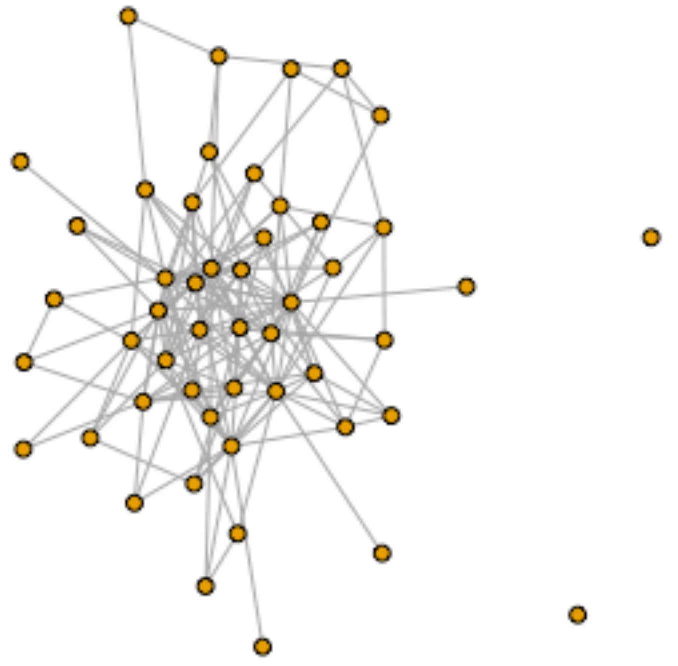
A sample from a dense mixture





Sample dense graph

G_{n_d}



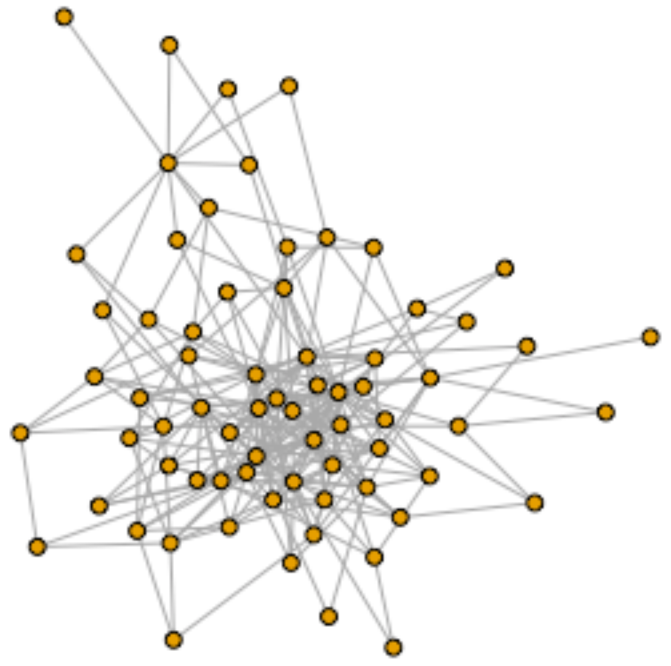
Sample sparse graph

$G_{n_s} = L^{-1}(H_{m_s})$

First sample disjoint cliques

Then compute the inverse line graph

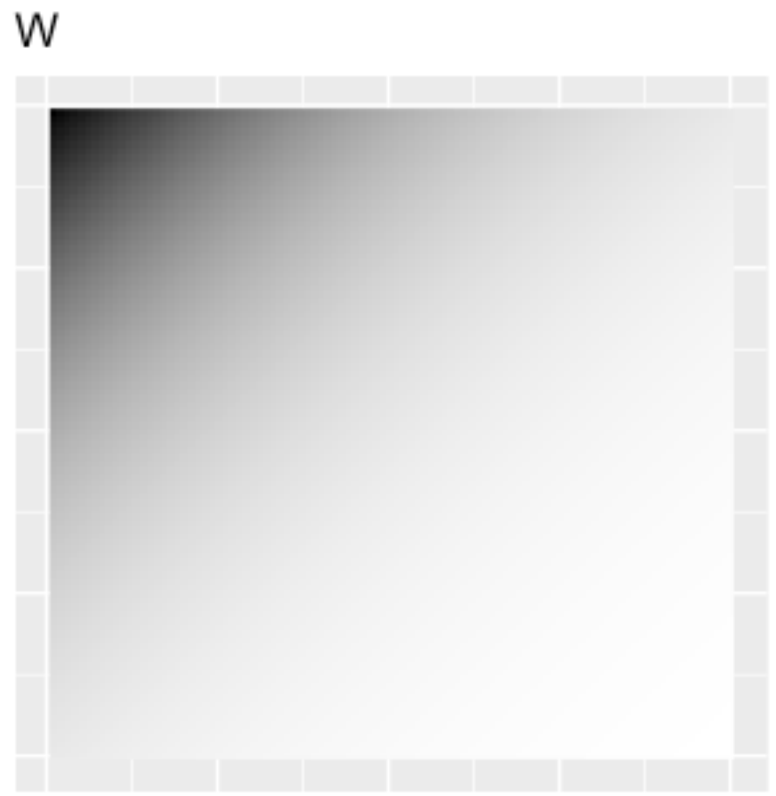
Mixture graph after joined

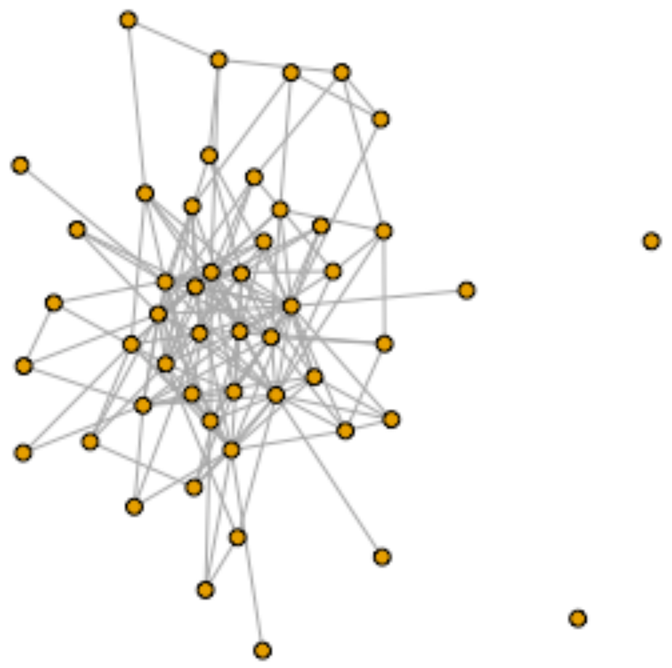


Bigger dense part

- $n_{d_i} = 50, n_{s_i} = 20$

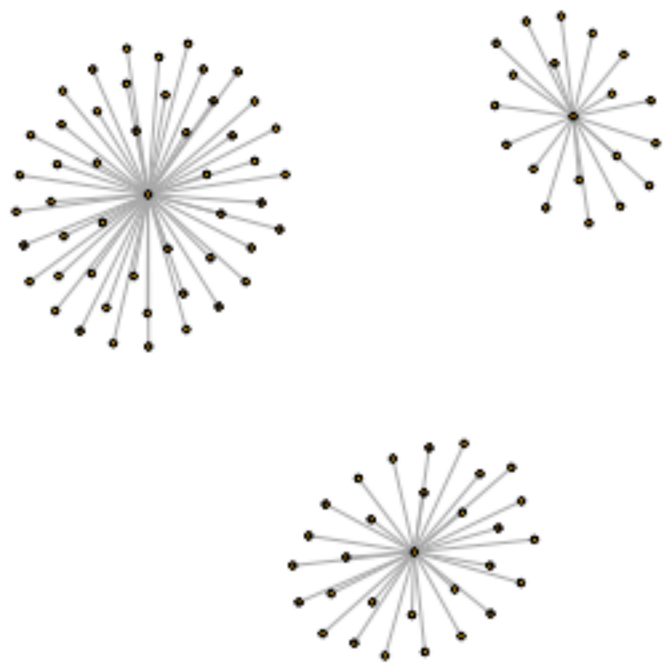
A sample from a sparse mixture

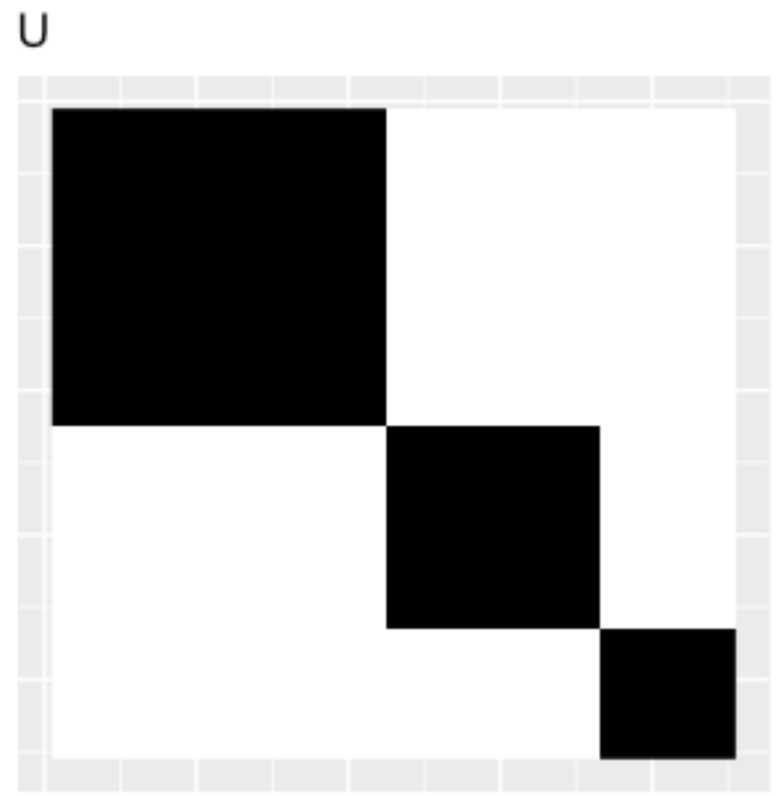




Sample dense graph

G_{n_d}





Bigger sparse part

Sample sparse graph

$G_{n_s} = L^{-1}(H_{m_s})$

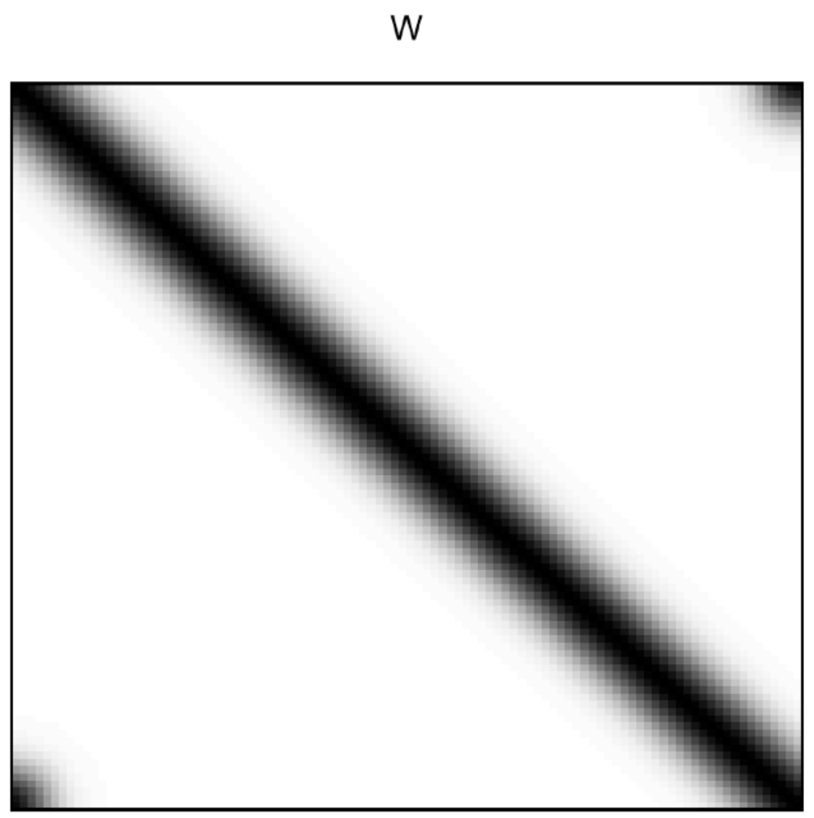
First sample disjoint cliques

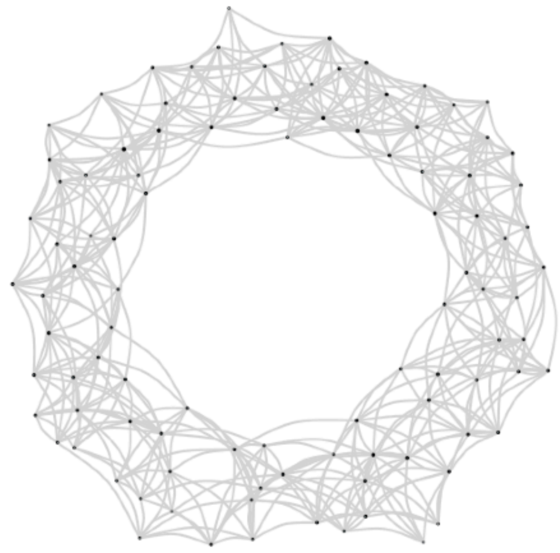
Then compute the inverse line graph

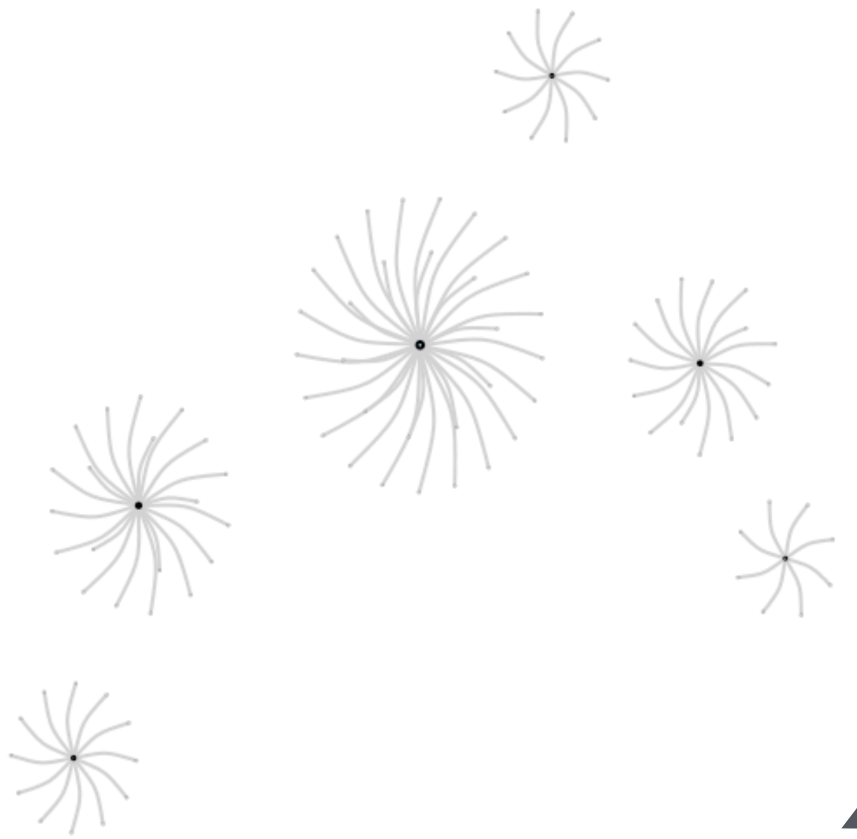
Mixture graph after joined

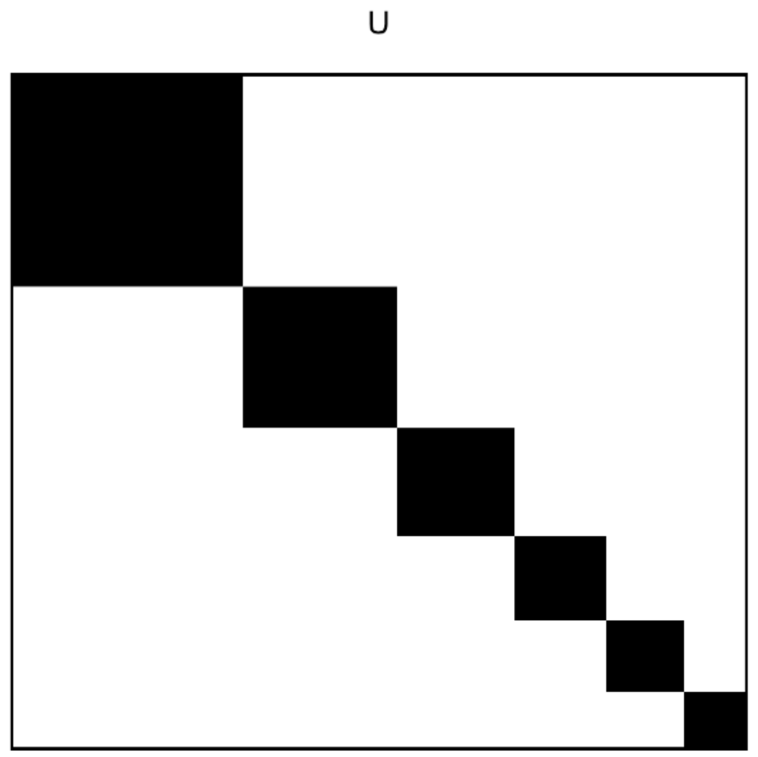
- $n_{d_i} = 50, n_{s_i} = 100$

A sample from a dense mixture









Sample dense graph

G_{n_d}

Bigger dense part

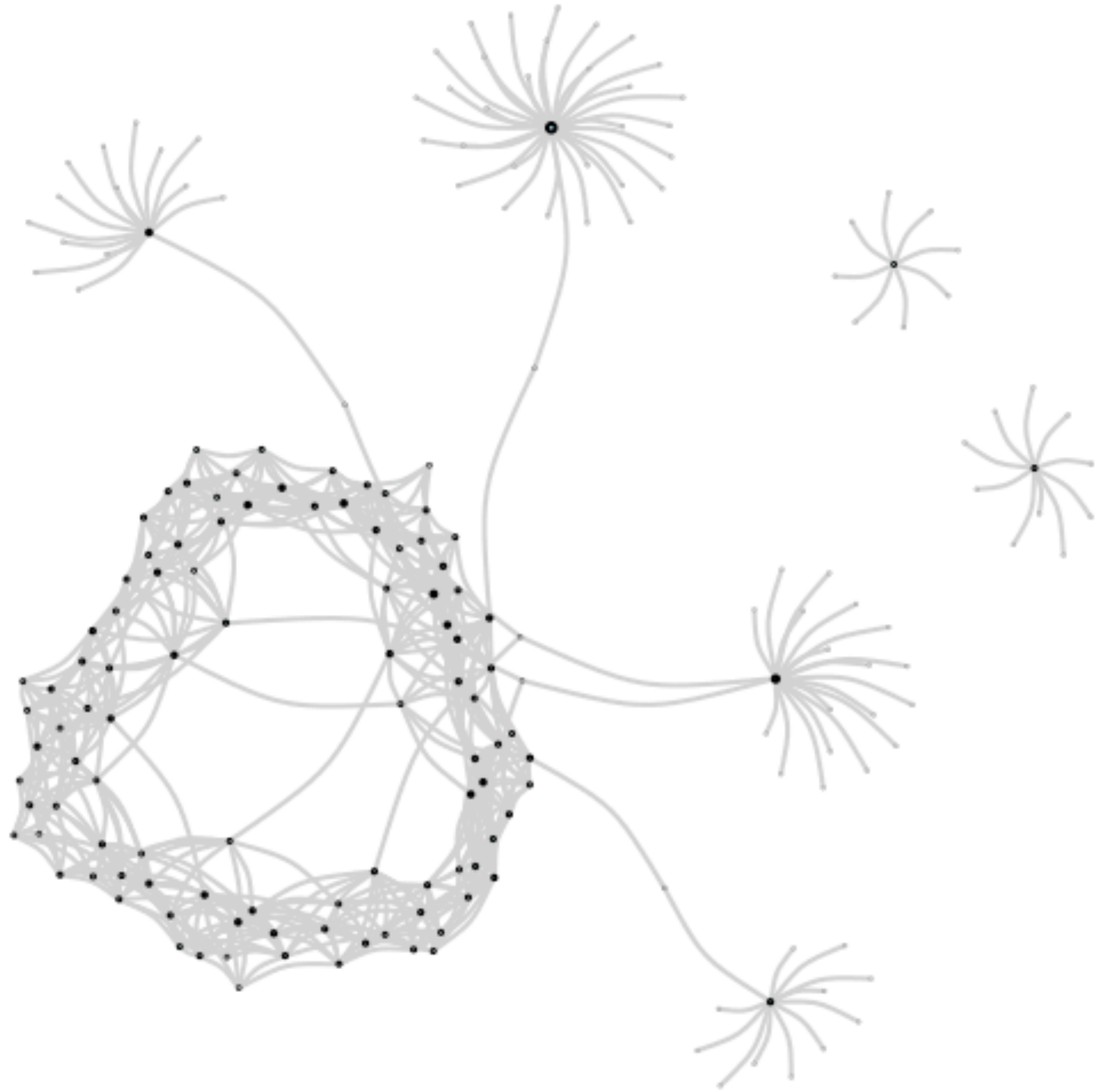
Sample sparse graph

$G_{n_s} = L^{-1}(H_{m_s})$

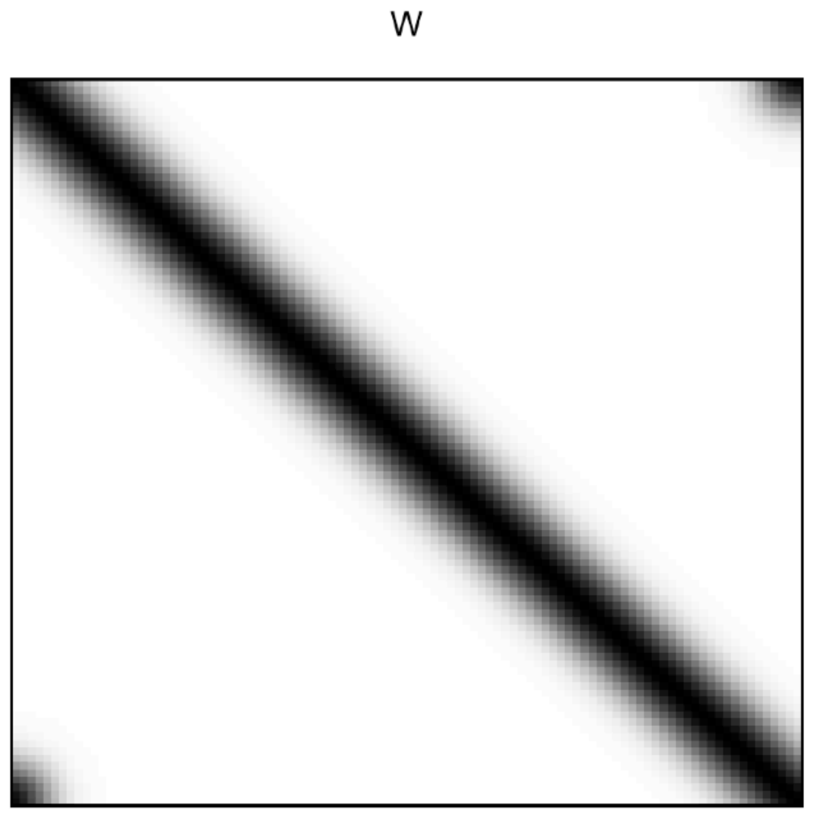
First sample disjoint cliques

Then compute the inverse line graph

Mixture graph after joined

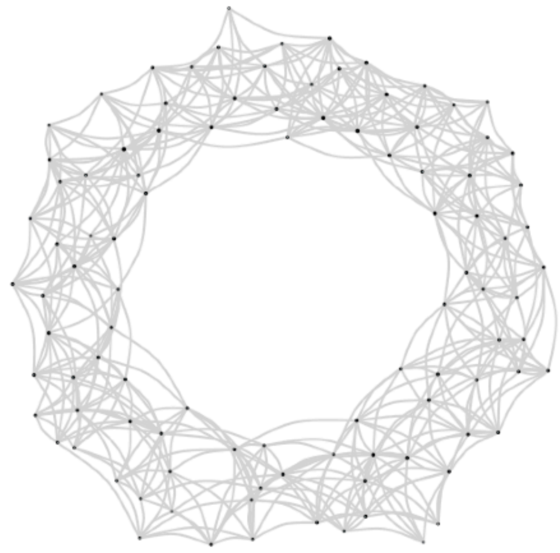


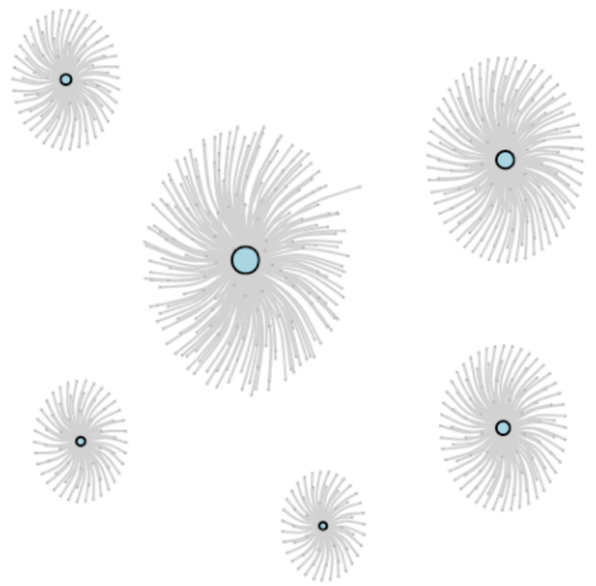
A sample from a sparse mixture

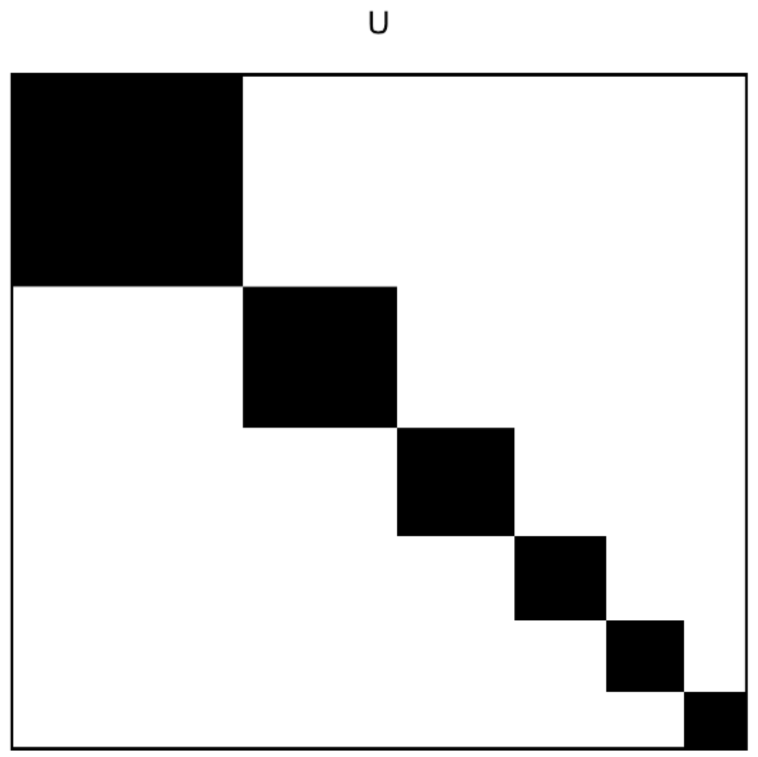


Sample dense graph

G_{n_d}







Bigger sparse part

Sample sparse graph

$G_{n_s} = L^{-1}(H_{m_s})$

First sample disjoint cliques

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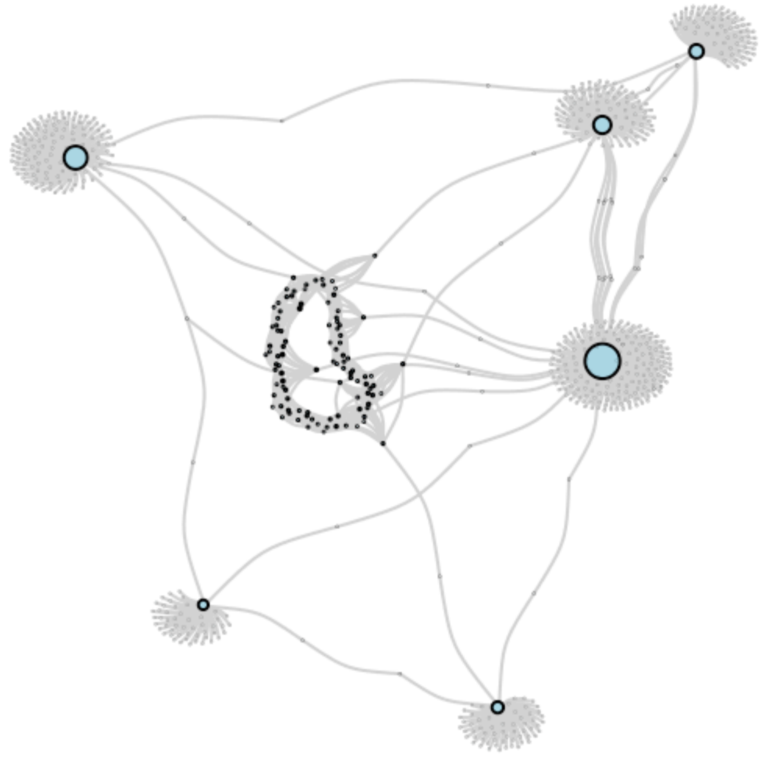
Mixture graph after joined



(U, W) graph mixtures can be dense or sparse

- $\{n_{d_i}\}_i$ - node num. sequence for dense part, $\{n_{s_i}\}_i$ - node number sequence for sparse part

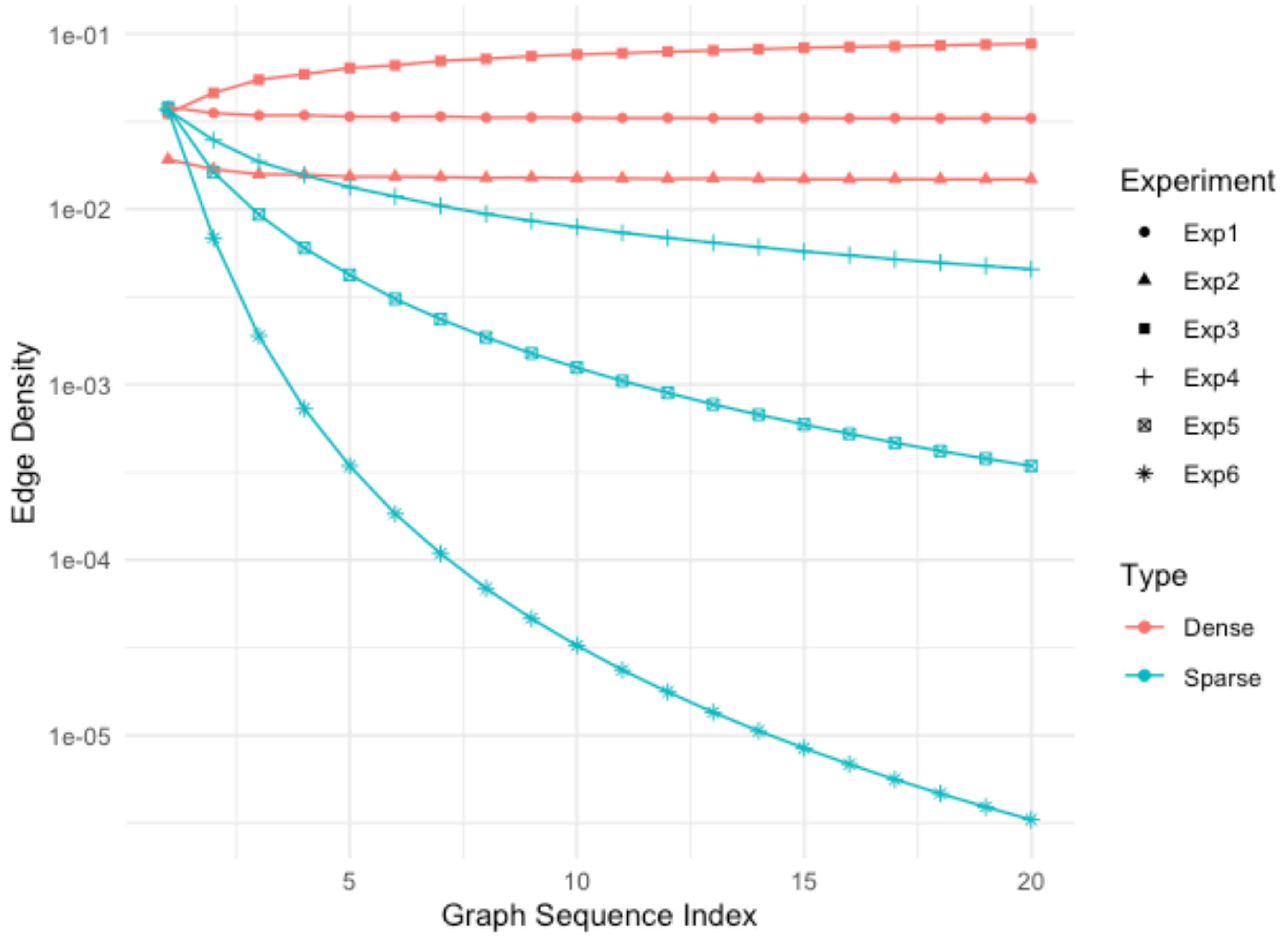
$$\lim_{i\to\infty} \frac{n_{s_i}}{n_{d_i}}$$

$$\lim_{i\to\infty} \frac{n_{s_i}}{n_{d_i}} = c < \infty$$

$\{G_{n_i}\}_i$ is dense

$$\lim_{i\to\infty} \frac{n_{s_i}}{n_{d_i}} = \infty$$

$\{G_{n_i}\}_i$ is sparse

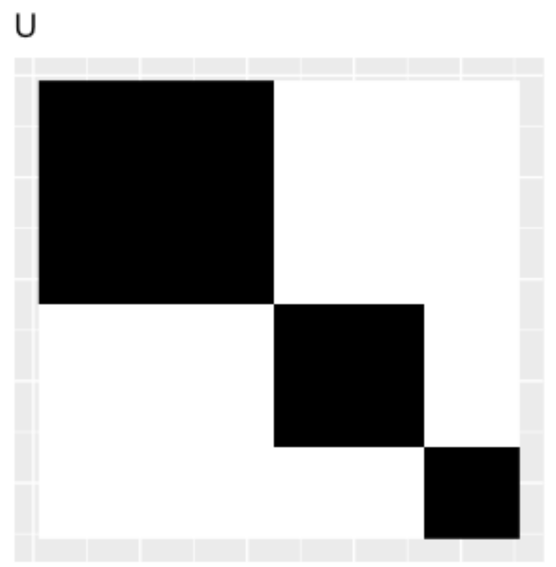


Inference

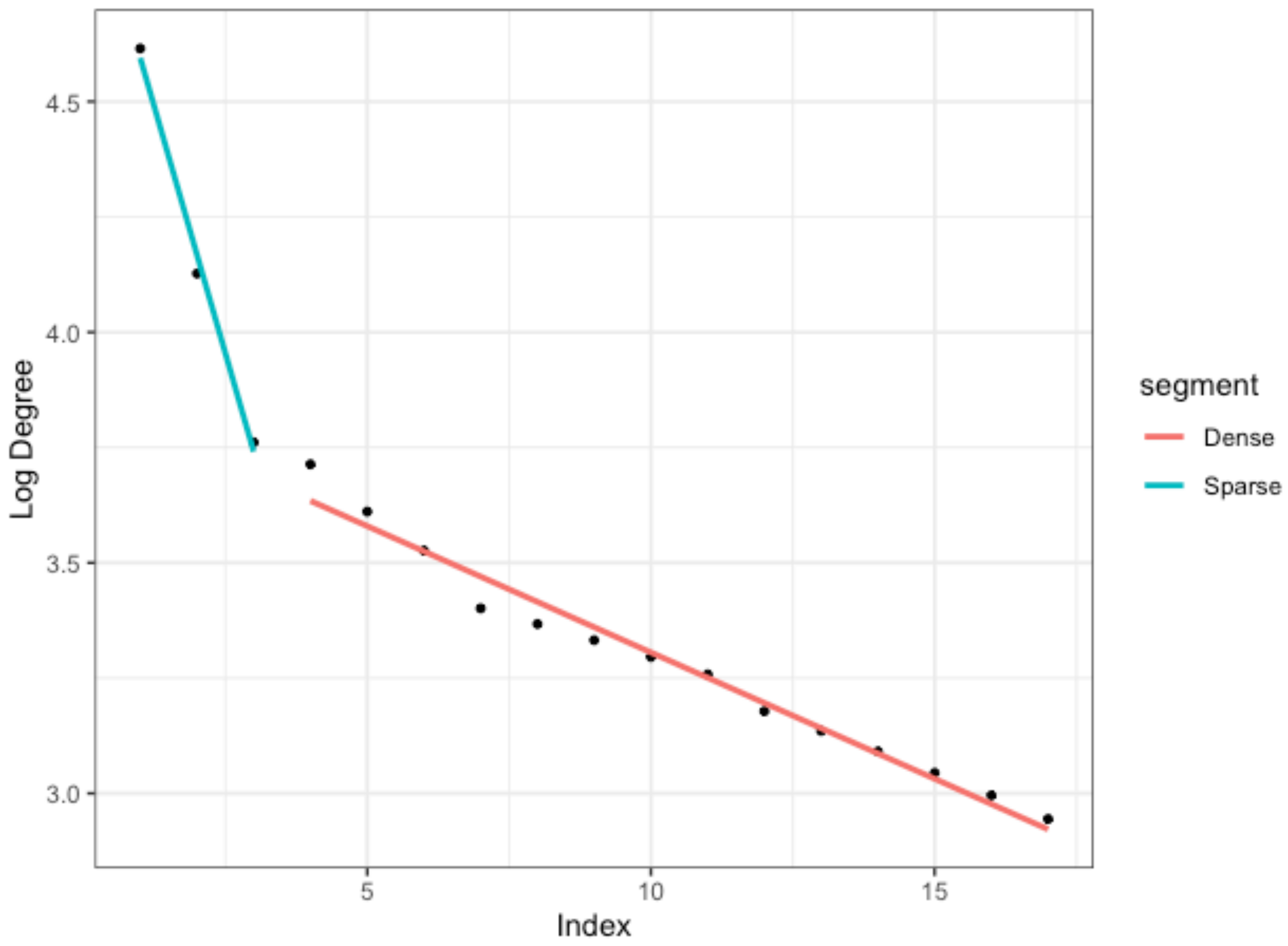
Inference and prediction

- Given a (U, W)-mixture graph, can we estimate U?
- Many methods to estimate W. The new part is U, that's our interest.
- We can estimate U, **if the graph sequence is sparse.**
- The degree distribution has the clue

Estimating $\boldsymbol{U}$ for sparse graphs



- By finding the elbow point we can estimate U
- U given by $\mathbf{p} = (p_1, p_2, \ldots)$ such that $\sum p_i = 1$
- $\hat{p}_j = \dfrac{q_j}{\sum_{i=1}^{\hat{k}} q_i}$, where q_i is the degree of the ith largest degree
- $\hat{k}$ is found from the elbow point



$$\left|\mathbb{E}(\hat{p}_j) - p_j\right| \leq \frac{c}{m_{s_i}} \quad \text{and} \quad \mathrm{Var}(\hat{p}_j) \leq \frac{c}{m_{s_i}}$$

Finite and infinite partitions of $\boldsymbol{U}$

$$
\begin{tikzcd}
 & U \arrow[dl] \arrow[dr] & \\
\mathbf{p} = (p_1, \ldots p_k) & & \mathbf{p} = (p_1, p_2, \ldots)
\end{tikzcd}
$$

$\hat{k} = k$ when graphs are large

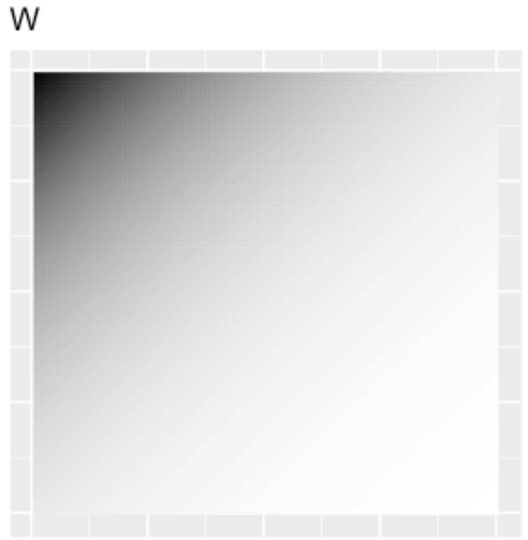
$\hat{k}$ increases as graphs grow in size

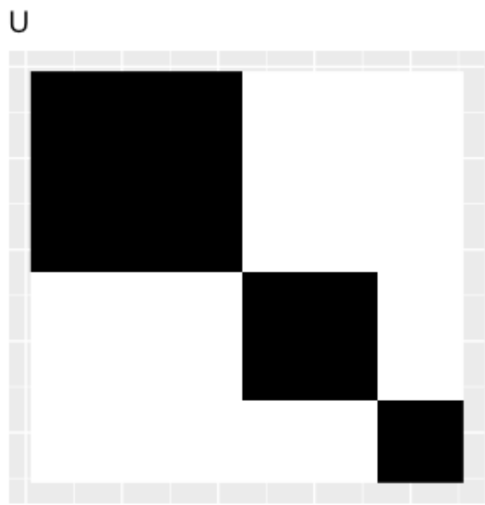
- U or $\mathbf{p} = (p_1, p_2, \ldots)$ gives the big players influence
- Eg - electricity network, if such a node is attacked, large negative impact

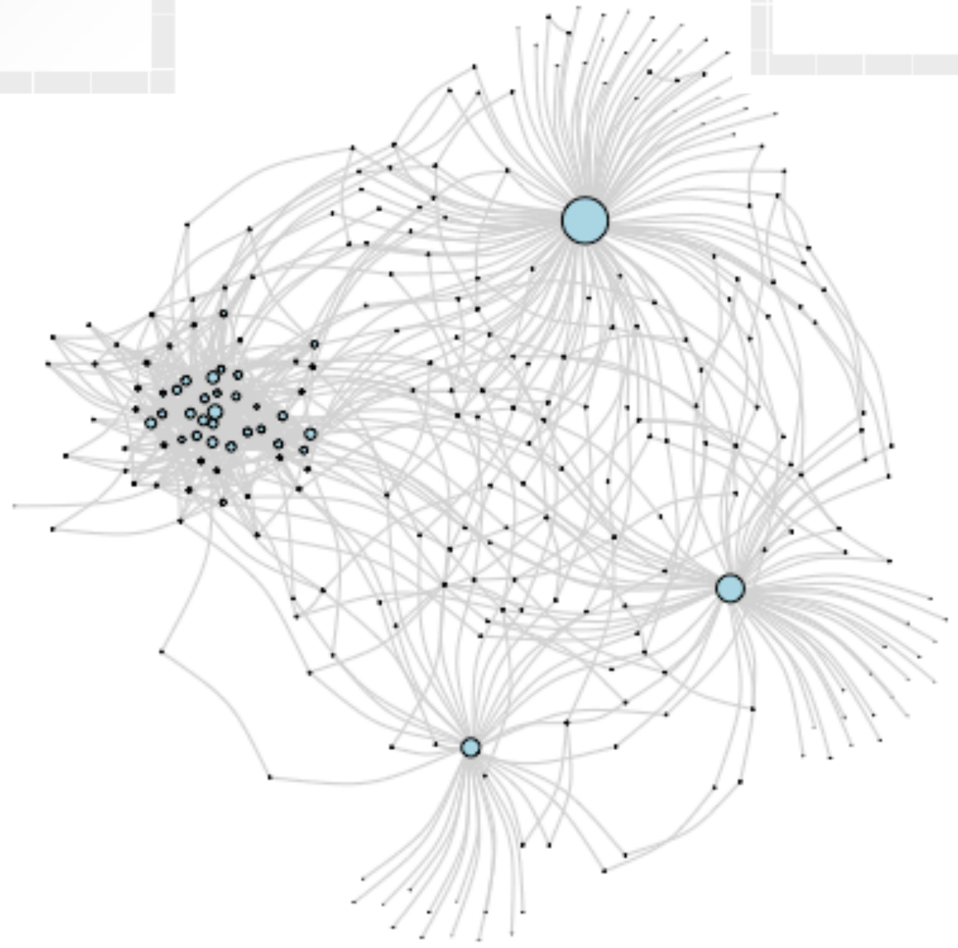
Top-k degrees of sparse (U, W) mixtures

- Hubs grow linearly with the total number of nodes n_i
- Say you observe graph G_{n_i} and you want to predict the hubs in G_{n_j} with $n_j > n_i$
- The degree of the kth hub $q_{k,i} \approx p_k m_{s_i}$ => $\hat{q}_{k,j} \approx q_{k,i} \frac{m_{s_j}}{m_{s_i}} \approx q_{k,i} \frac{n_{s_j}}{n_{s_i}}$

(U, W) graphon mixtures







- Simpler method to generate sparse graphs using inverse line graphs

- Generate dense and sparse graphs from W and U and join them

- Typical real networks have high degree hubs forming the skeleton with low degree vertices constituting the body of the network

- Sparse (U, W) mixture graphs have this property

- Flexibility: depending on how n_{s_i}/n_{d_i} increase, we can get dense or sparse graphs

- We can infer U and predict the top-k degrees of unseen sparse graphs with some guarantees

Future work

- What about other types of joins? (We've used random joining)
- Other sparse graphs - paths, rings, isolated edges . . . (not the driving force of social network graphs but . . .)
- R package - `graphonmix` - https://github.com/sevvandi/graphonmix
- Topic post

Thank you!

Questions?