Graphons, mergeons, and so on!

Justin Eldridge

with

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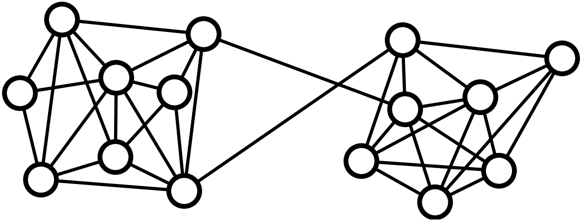
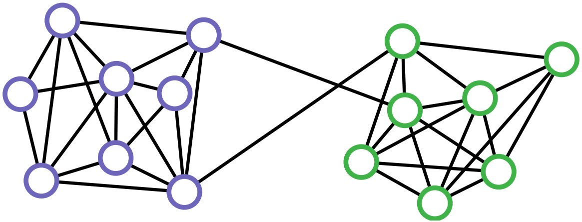
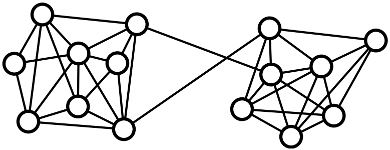
The Ohio State University

Graph clustering



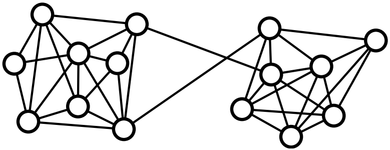
Graph clustering





Question 1

What is the "correct" clustering of the graph?



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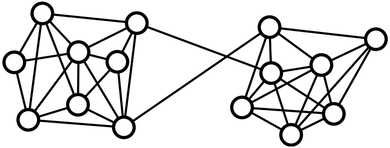

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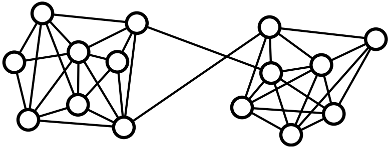

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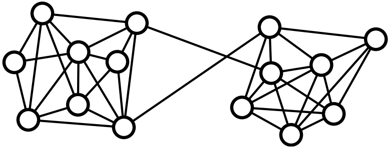

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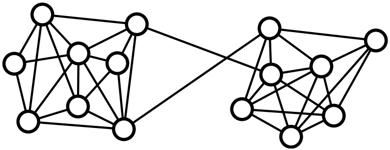
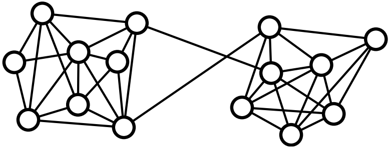
- Define the clusters of the model itself.



Question 1

What is the "correct" clustering of the graph?

- There is no single answer.
- Right answer depends on nature of the data.
- When graph generated from a random graph model...
- Define the clusters of the model itself.
- Goal of clustering: recover the clusters of the model from a single graph.



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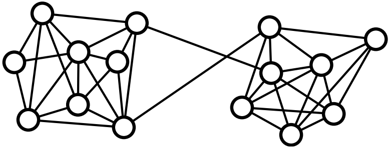
What does it mean to recover the “correct” clustering?



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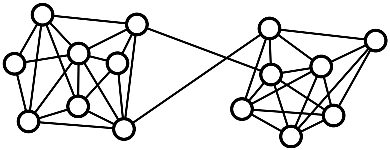
What does it mean to recover the “correct” clustering?

- Need a notion of statistical consistency for the clusters of the random graph model.



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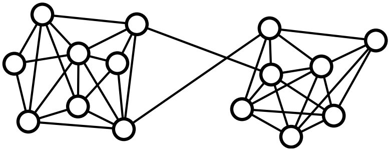
How do we recover the correct clustering?



Question 2

What does it mean to recover the “correct” clustering?

- Need a notion of statistical consistency for the clusters of the random graph model.

Question 3

How do we recover the correct clustering?

- Do correct algorithms exist?

In this talk...

We assume a very general and powerful random graph model called a graphon.

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Question 1: What is the “correct” clustering of a graphon?

- We introduce the graphon cluster tree.
- Introduce a useful encoding which we call a mergeon.

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Question 3: How do we recover the graphon cluster tree?

- We give sufficient conditions under which a graphon estimator leads to a correct clustering method.
- We identify a practical, correct clustering algorithm.

What is a graphon?

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

- Intuitively: the weight matrix of a graph on node set $[0,1]$.

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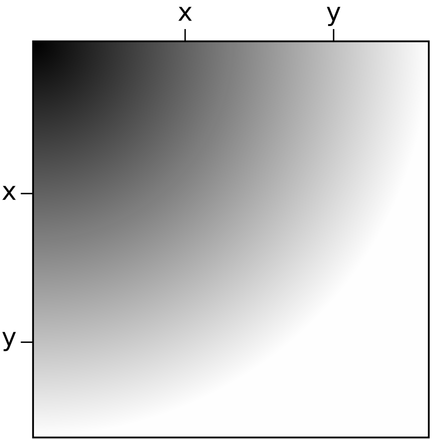

A graphon's "nodes" are points in $[0,1]$.

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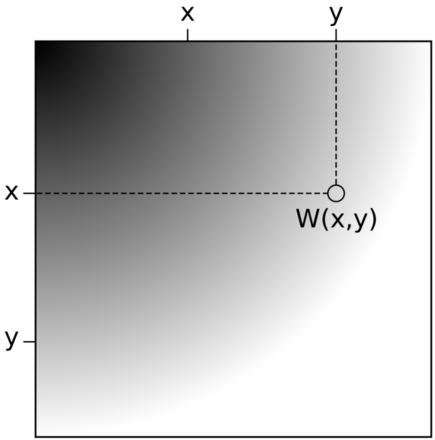

The weight of the "edge" (x, y) is $W(x, y)$.

A graphon is a rich object...

Large networks and graph limits

László Lovász

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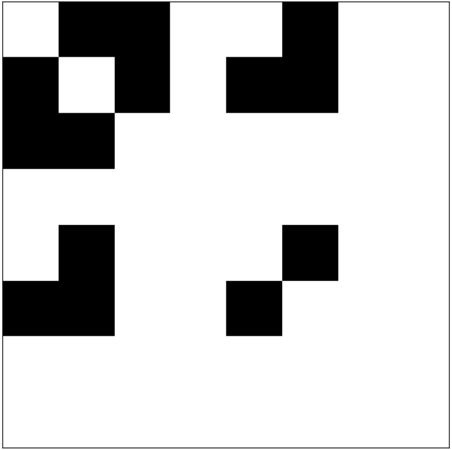
A graphon is a graph limit.



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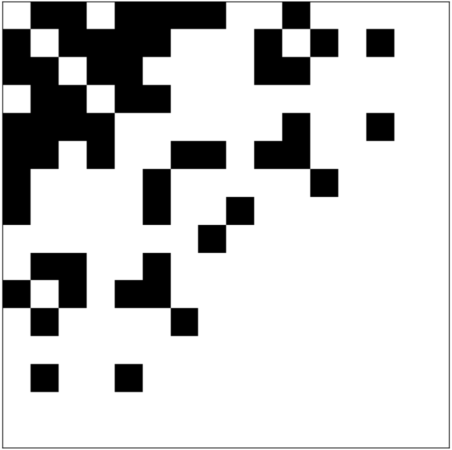

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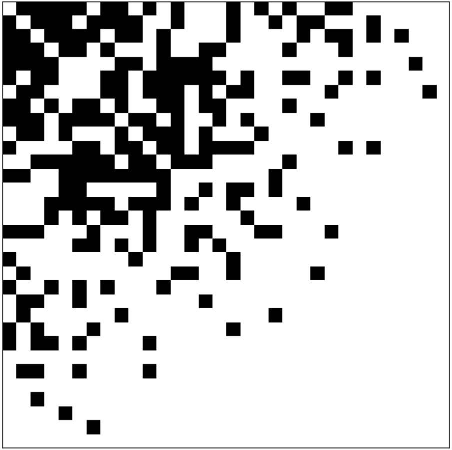

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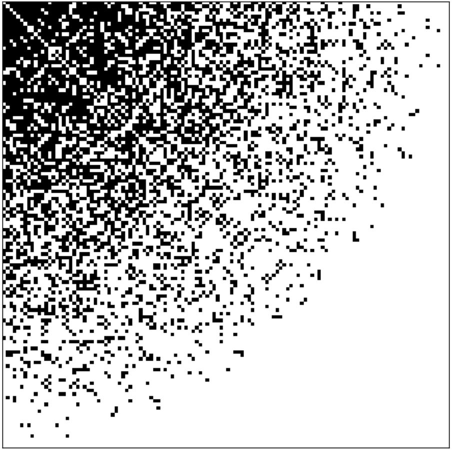

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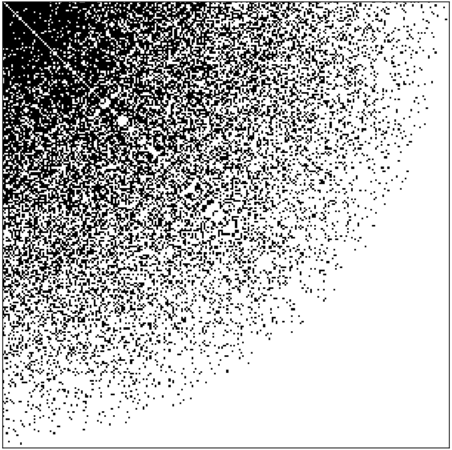

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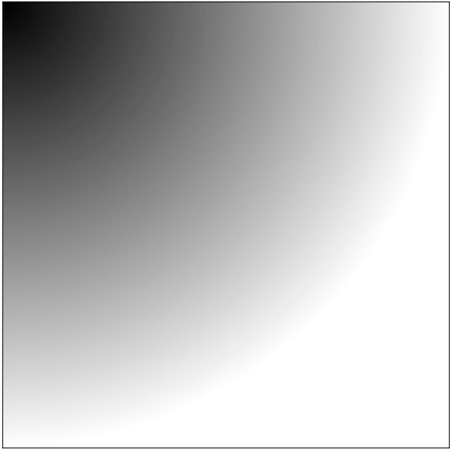
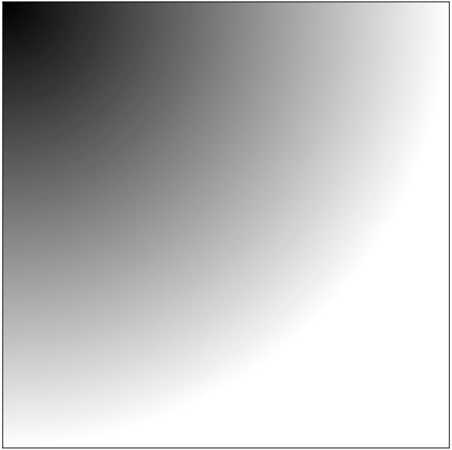
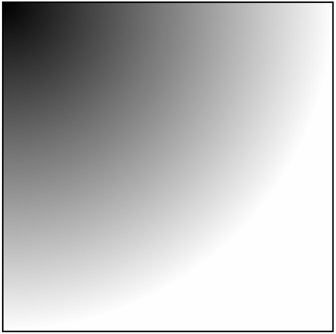


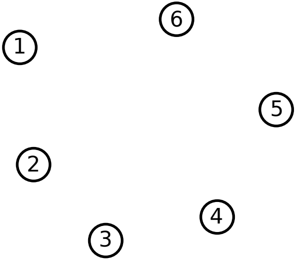
A graphon is a random graph model.



When $W(x, y)$ is interpreted as a probability.

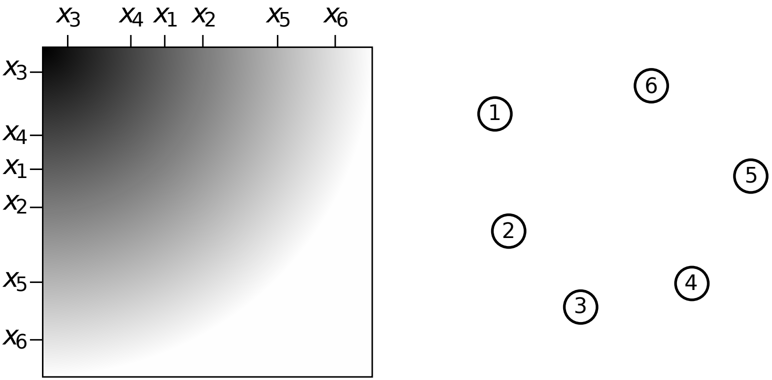
Sampling from a graphon





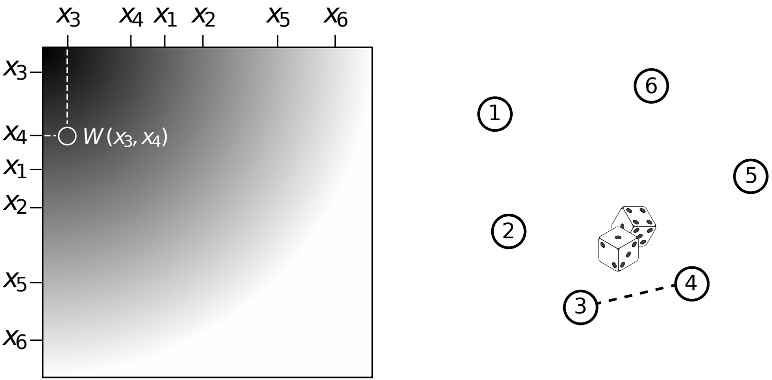
Start with a graph with integer node set [n].

Sampling from a graphon



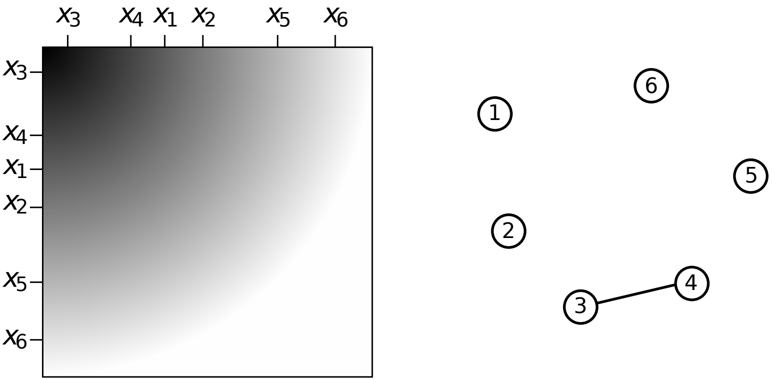
Draw n points $\{x_1, \ldots, x_n\}$ from Unif([0, 1]).

Sampling from a graphon



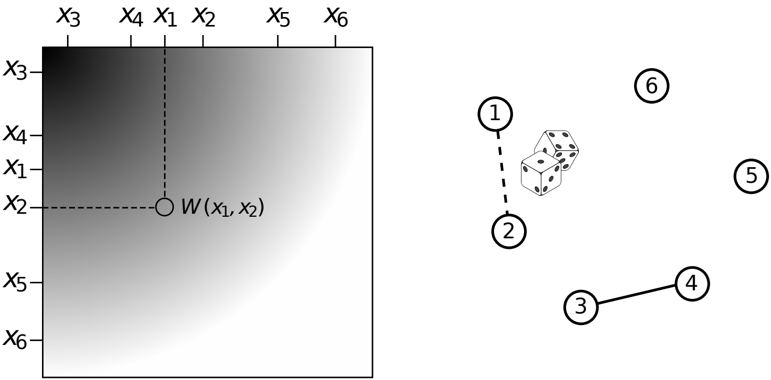
Connect nodes 3 and 4 with probability $W(x_3, x_4)$.

Sampling from a graphon



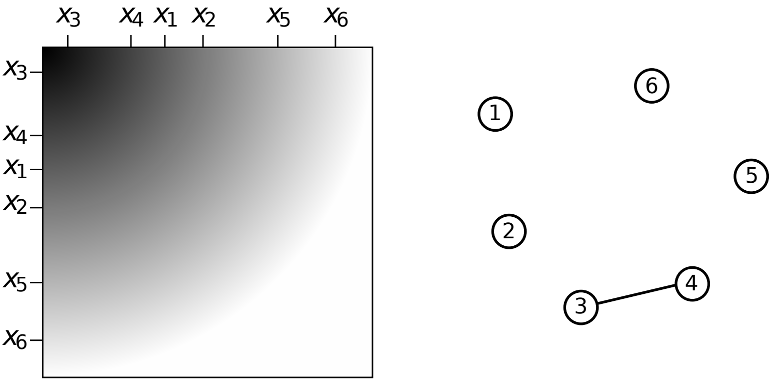
By chance, edge $(3, 4)$ is included.

Sampling from a graphon



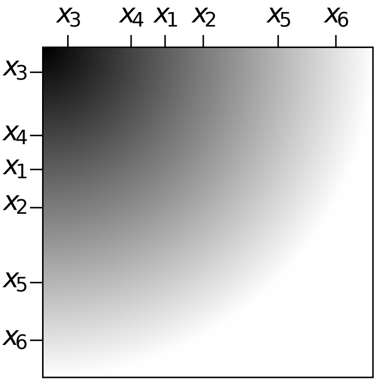
Connect nodes 1 and 2 with probability $W(x_1, x_2)$.

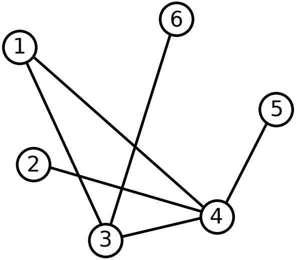
Sampling from a graphon



By chance, edge $(1, 2)$ is omitted.

Sampling from a graphon





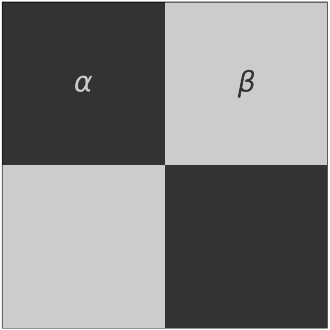
Repeat for all edges, resulting in a randomly-generated graph.

The stochastic blockmodel

Much theory of graph clustering assumes a stochastic blockmodel. Example:

- Randomly assign each of n nodes to one of two communities.
- Add edge between two nodes with probability:
  - α, if in the same community,
  - β, otherwise.

This is a special case of a graphon.



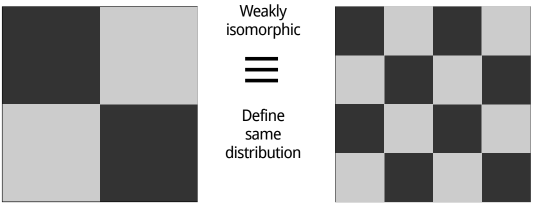
Equivalent graphons

- Any graphon W defines a distribution on graphs.
- Not uniquely! Many graphons define the same distribution.

Equivalent graphons

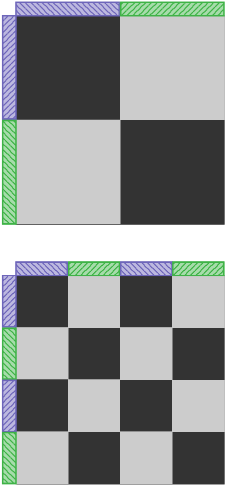
- Any graphon W defines a distribution on graphs.
- Not uniquely! Many graphons define the same distribution.
- Graphs are isomorphic if they are equivalent up to relabeling.
- Graphons are weakly isomorphic if they are equivalent up to a relabeling $\varphi : [0, 1] \to [0, 1]$.
  - φ must be measure preserving.
- An equivalence class of graphons under weak isomorphism uniquely defines distribution.

W $\qquad$ $W^{\varphi}, \varphi = 2x \mod 1$

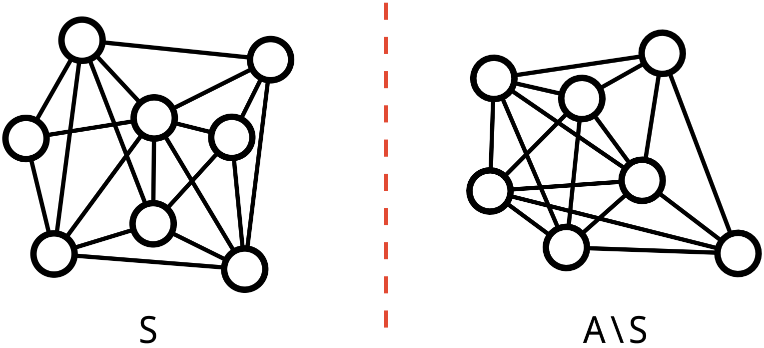


Question 1: What are the clusters of a graphon?

- It is natural to define clusters in terms of connected components.
- Carefully define connectivity for graphons.
- Intuitively: blockmodel graphon should have the two clusters shown.
- Clusters should be:
  - robust to changes to W on a set of zero measure,
  - preserved under relabeling of W.

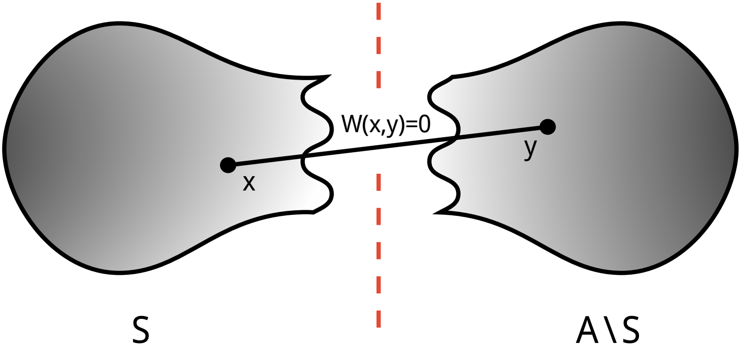


Connectedness in graphs



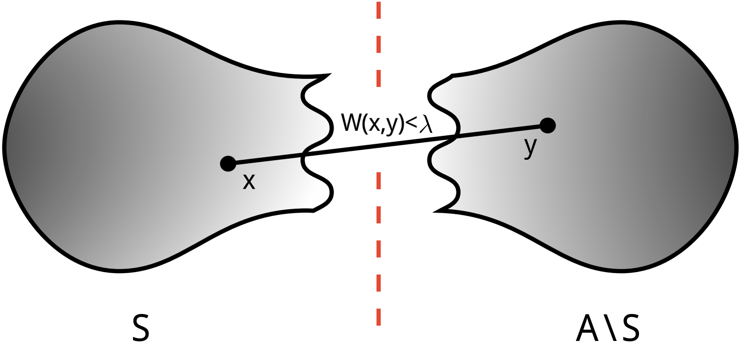
A is disconnected if it can be partitioned into S and A \ S with no crossing edge. Otherwise it is connected.

Connectedness in graphons

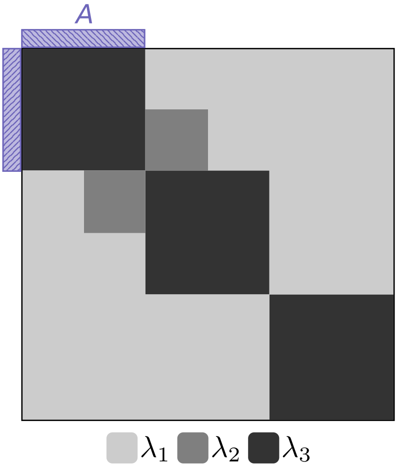


(Janson, 2008): A is disconnected if it can be partitioned into S and A \ S such that the weight of almost every crossing edge is zero. Otherwise it is connected.

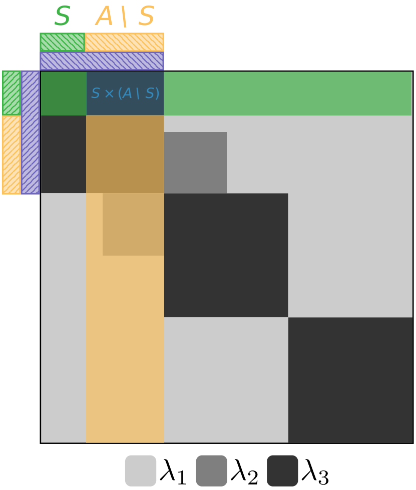
Connectedness in graphons



A is disconnected at level λ if it can be partitioned into S and A \ S such that the weight of almost every crossing edge is less than λ. Otherwise it is connected at level λ.



Connected at level λ_3.



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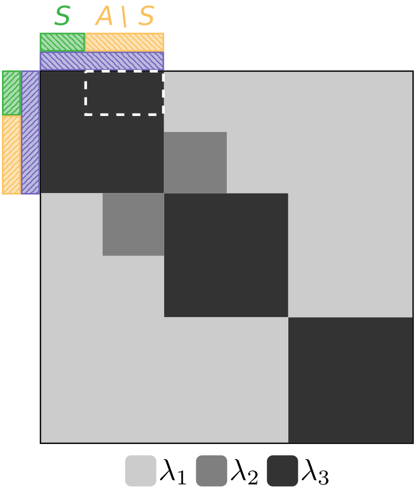

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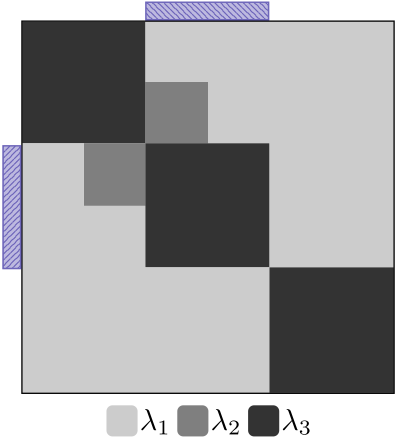

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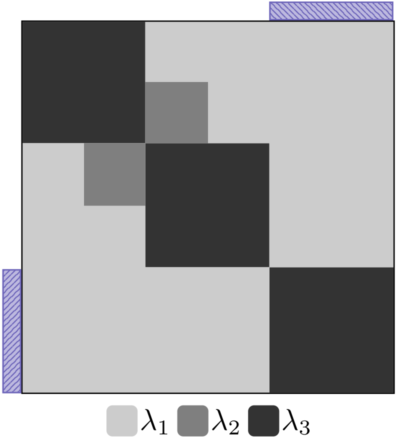

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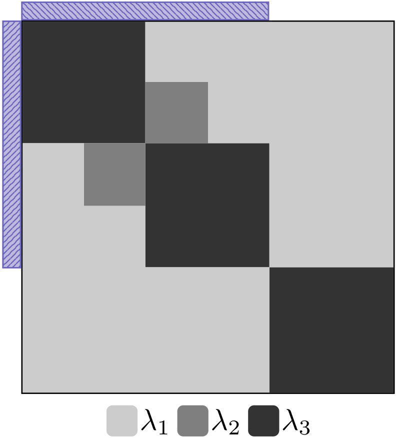
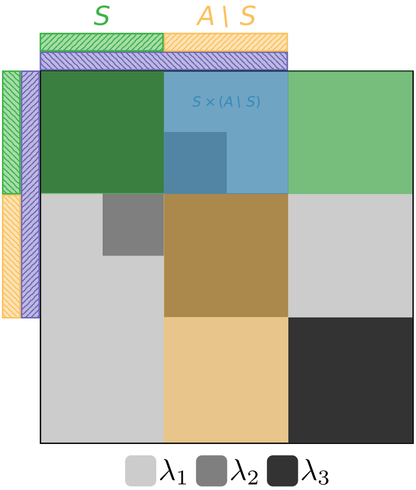


Disconnected at level λ_3.



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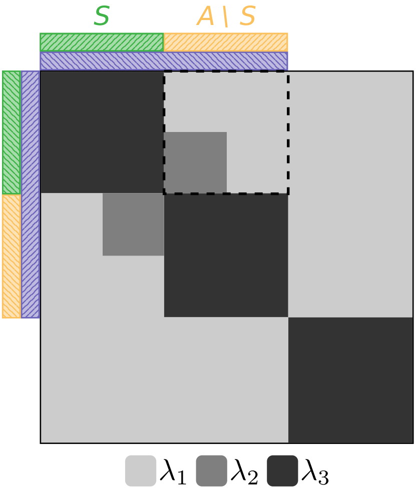

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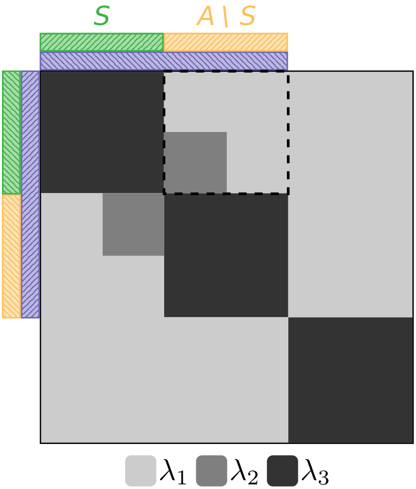
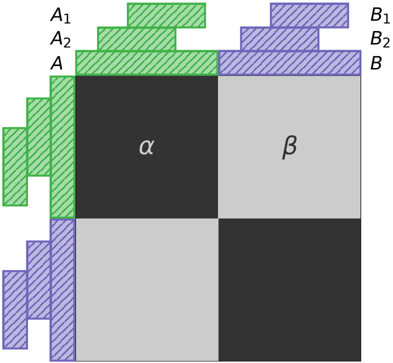


Connected at level λ_2.

The clusters of a graphon

Naturally define clusters in terms of maximally connected sets:



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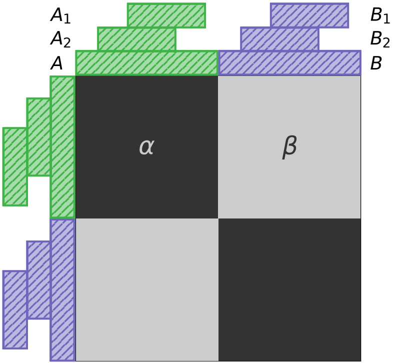

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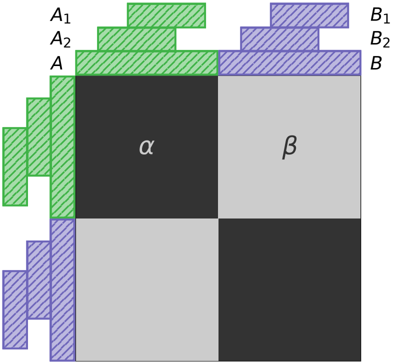

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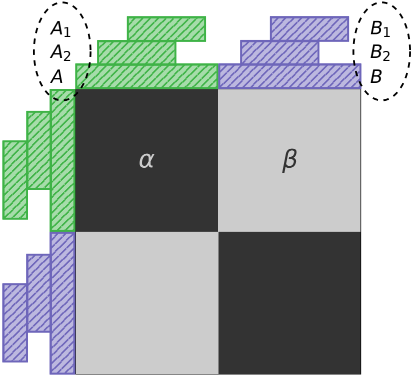

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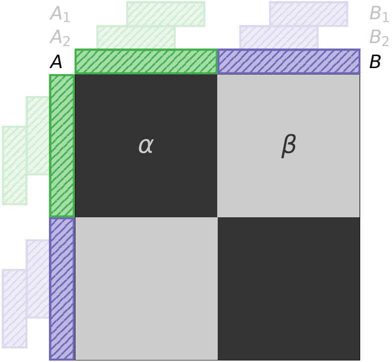

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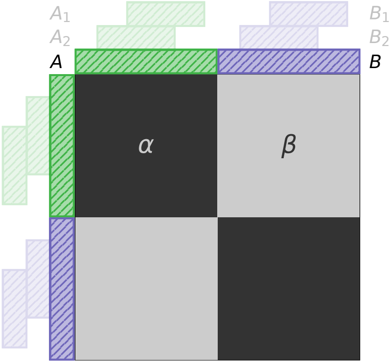
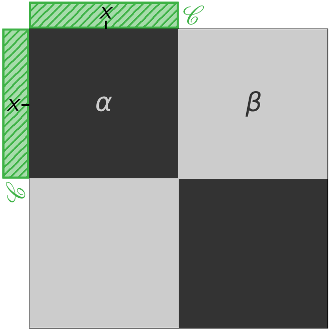


We write $\mathbb{C}_W(\lambda)$ to denote the set of clusters of W at level λ.

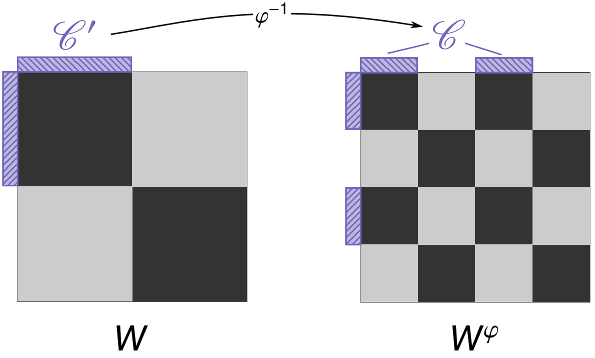
Properties of clusters

- Connectivity of a set is not changed by adding/removing sets of zero measure.
- Careful! A cluster $\mathscr{C} \in \mathbb{C}_W(\lambda)$ is not a subset of $[0,1]$!
  - It is an equivalence class of subsets equal up to null sets.
  - A single point $x \in [0,1]$ belongs to no cluster in particular.



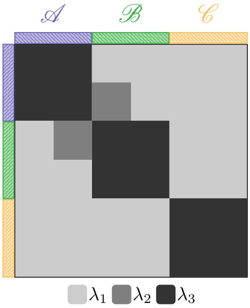
Properties of clusters

- Claim: Clusters are preserved under relabelings.
- I.e., the clusters of a graphon W and the clusters of its relabeling W^{φ} are in bijection.
  - Surprisingly non-trivial to show due to graphon subtleties.
- Example: $\varphi(x) = 2x \mod 1$



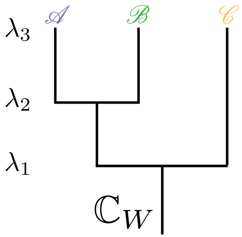
The graphon cluster tree

- The set of clusters $\mathbb{C}_W$ from all levels has hierarchical structure.
  - I.e., if C and C′ are clusters, then either $\mu(C \cap C') = 0$, $\mu(C \setminus C') = 0$, or $\mu(C' \setminus C) = 0$.
- We call $\mathbb{C}_W$ the graphon cluster tree of W.
- Claim: If two graphons are equivalent, their cluster trees are isomorphic.



The goal of clustering (graphon setting)

- Given a graph sampled from W...
- recover the cluster tree of W.



Mergeons

- We may naturally speak of the height at which clusters merge.
- But the merge height of any pair of nodes is undefined.
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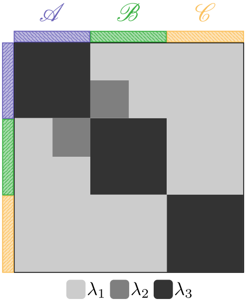
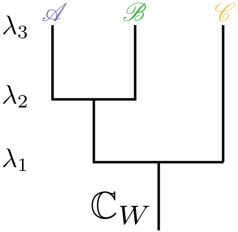
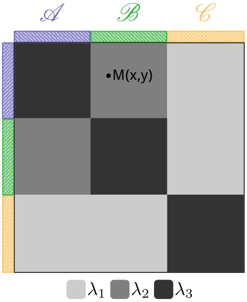


Graphon W





Mergeon M of W

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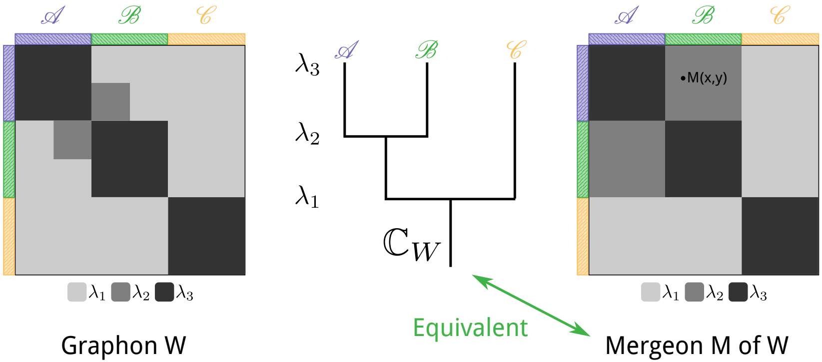

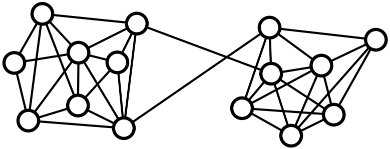

Question 1: What is the "correct" clustering of a graphon?
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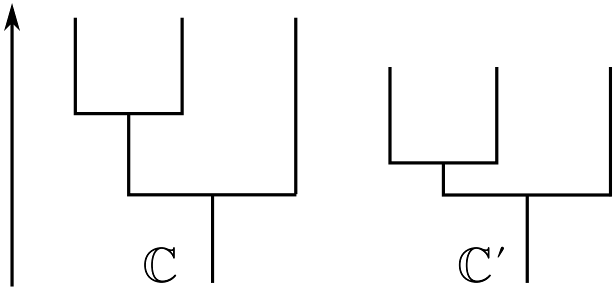
The merge distortion



How "close" are $\mathbb{C}$ and $\mathbb{C}'$?

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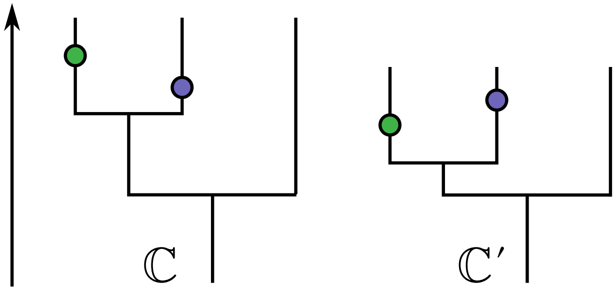

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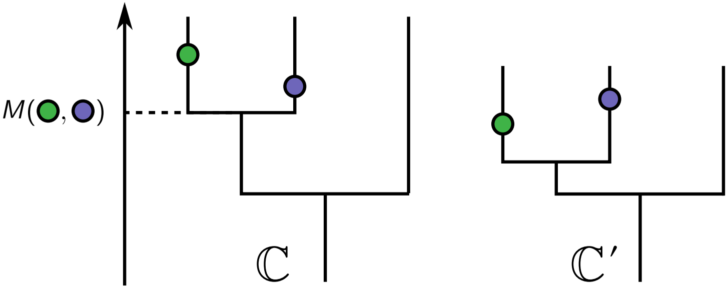

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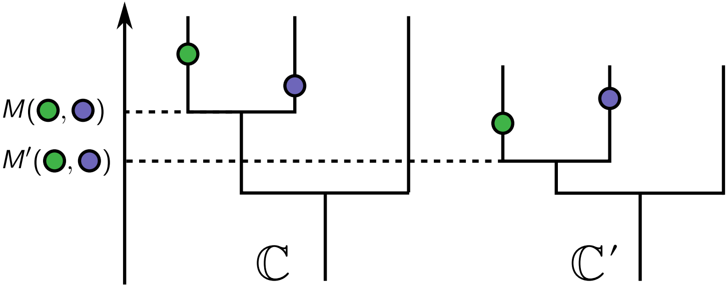

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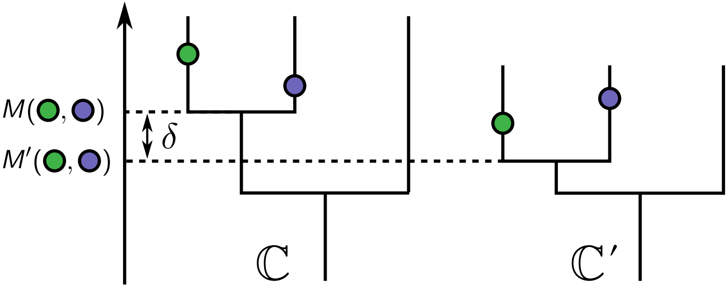

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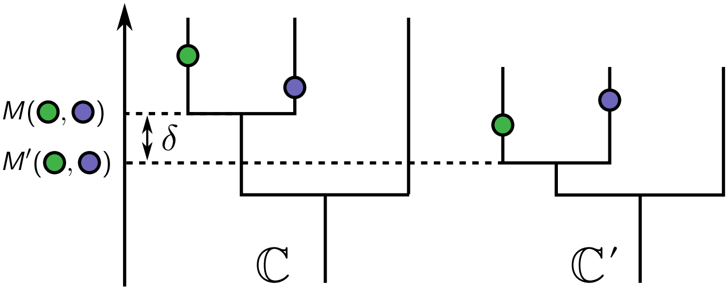


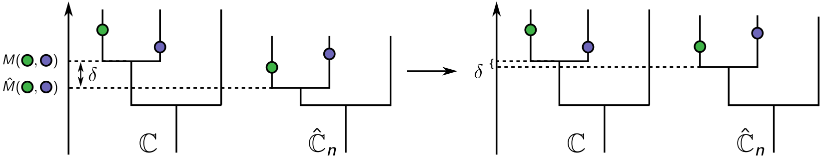
The merge distortion between $\mathbb{C}$ and $\mathbb{C}'$ with respect to a (finite) set S is:

$$d_S(\mathbb{C}, \mathbb{C}') = \max_{s_1 \neq s_2 \in S} \left| M(s_1, s_2) - M'(s_1, s_2) \right| .$$

Convergence in merge distortion

Definition

A sequence $\hat{\mathbb{C}}_n$ converges in merge distortion to $\mathbb{C}$ if $d(\mathbb{C}, \hat{\mathbb{C}}_n) \to 0$ as $n \to \infty$.



Consistent clustering methods

Question 2

What does it mean to recover the "correct" clustering?

- A clustering method is consistent for the graphon W if its output converges in merge distortion to $\mathbb{C}_W$, w.h.p. as $n \to \infty$.

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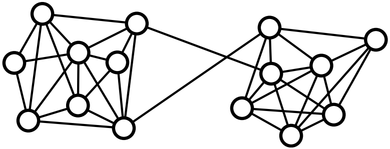
Question 2

What does it mean to recover the "correct" clustering?

- A clustering method is consistent for the graphon W if its output converges in merge distortion to $\mathbb{C}_W$, w.h.p. as $n \to \infty$.
- That is:
  - If G_n is a random graph of size n sampled from W,
  - $\hat{\mathbb{C}}_{G_n}$ is the output of the method given G_n as input,
  - then, for any fixed $\epsilon > 0$, $\mathbb{P}(d(\mathbb{C}_W, \hat{\mathbb{C}}_{G_n}) > \epsilon) \to 0$ as $n \to \infty$.
- Consistent methods recover the clusters of the graphon.



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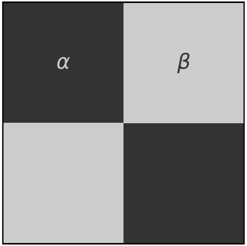
Question 2: What does it mean to recover the "correct" clustering?
Answer: Convergence in merge distortion to graphon cluster tree.

Question 3: How do we recover the correct clustering?

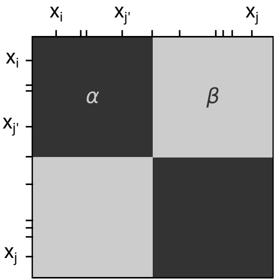
- I.e., do algorithms exist which are consistent in merge distortion?

Estimating edge probabilities



Consider sampling a graph from this graphon.

Estimating edge probabilities



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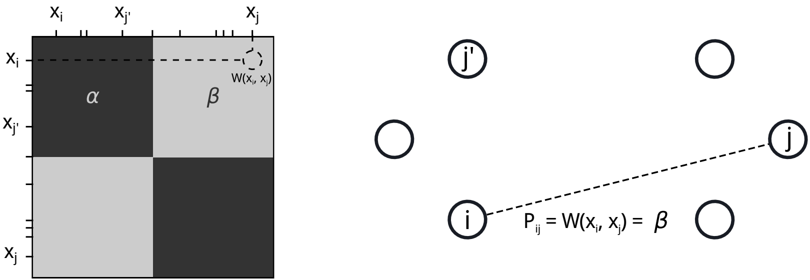

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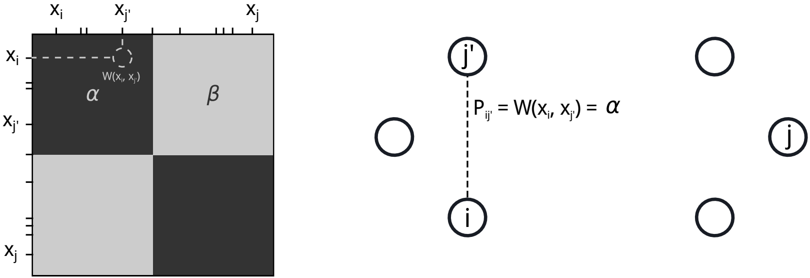

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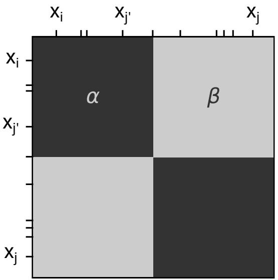
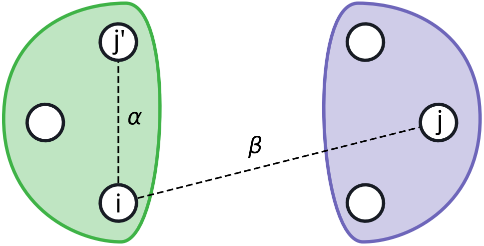
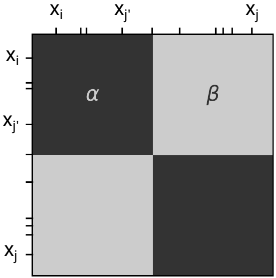
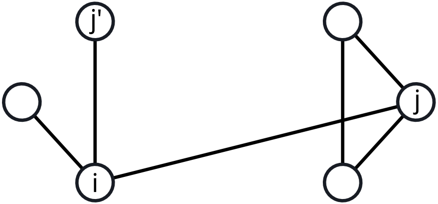




The correct clustering is determined by these edge probabilities.

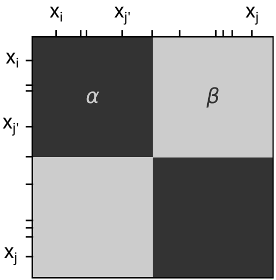
Estimating edge probabilities

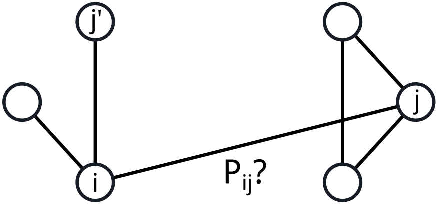




But the edge probabilities are unknown, and the presence of an edge (i, j) tells us little about P_{ij}.

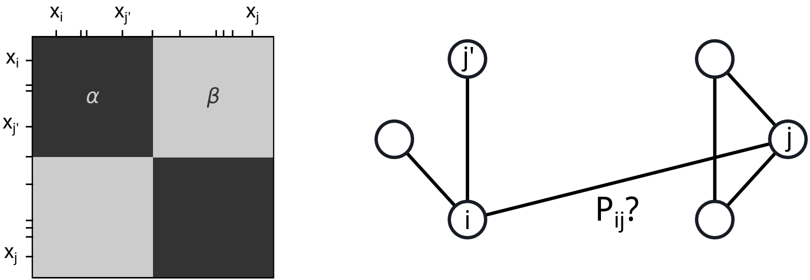
Estimating edge probabilities





Goal: Compute estimate $\hat{P}$ of edge probabilities from single graph.

Estimating edge probabilities



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Theorem

If $\|P - \hat{P}\|_\infty \to 0$ in probability as $n \to \infty$, then single linkage clustering on $\hat{P}$ is a consistent clustering method.

Neighborhood smoothing

- To cluster consistently, it is sufficient to estimate P in ∞-norm.
- We now search for such an estimator...
- Zhang et al. (2015) propose neighborhood smoothing.

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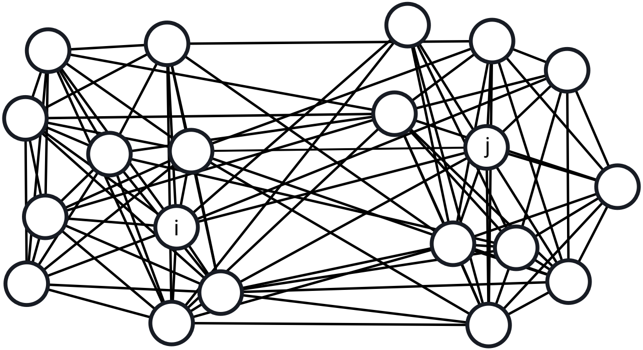
  - But we have just one observation.
- Approach:
  - For node i, build neighborhood N_i of similar nodes.
  - Think of $i' \in N_i$ as another observation of i.
  - To estimate P_{ij}: count number of edges between j and a node in N_i.

Neighborhood smoothing



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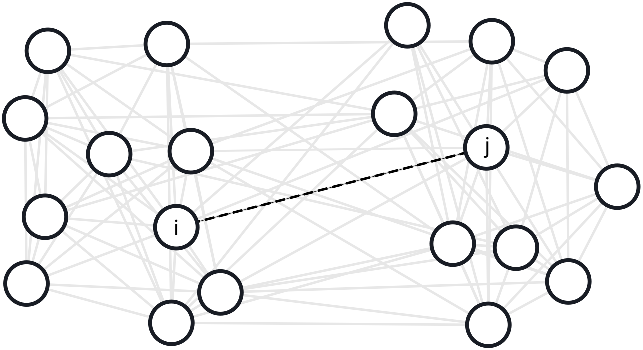

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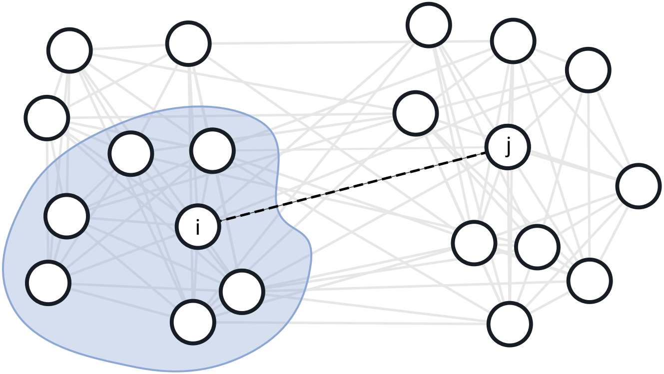
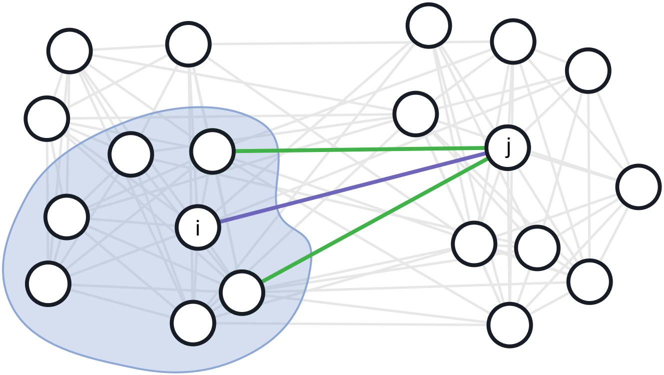


Build a neighborhood N_i of nodes with similar connectivity to that of i. I.e., close in the distance: $d(i, i') = \max_{k \neq i, i'} \left|(A^2)_{ik} - (A^2)_{i'k}\right|$.

Neighborhood smoothing



- Count number of edges from N_i to node j (excluding i): 2.
- Normalize by size of neighborhood: 6.
- Estimated edge probability: $\hat{P}_{ij} = {}^2/_6 = {}^1/_3$.

Consistency of neighborhood smoothing

- Zhang et al. (2015) prove that neighborhood smoothing is consistent in mean squared error:

$$\frac{1}{n^2}\|P - \hat{P}\|_F^2 = \frac{1}{n^2}\sum_{ij}(P_{ij} - \hat{P}_{ij})^2 \to 0 \quad \text{as} \quad n \to \infty, \text{ w.h.p.}.$$

- But convergence in this norm is too weak. We need convergence in ∞-norm.
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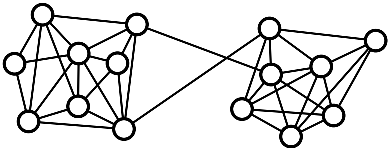
Theorem

The modified neighborhood smoothing estimator for P is consistent in ∞-norm.

Corollary

Performing single linkage on the modified neighborhood smoothing estimate of P is a consistent graphon clustering method.

Summary



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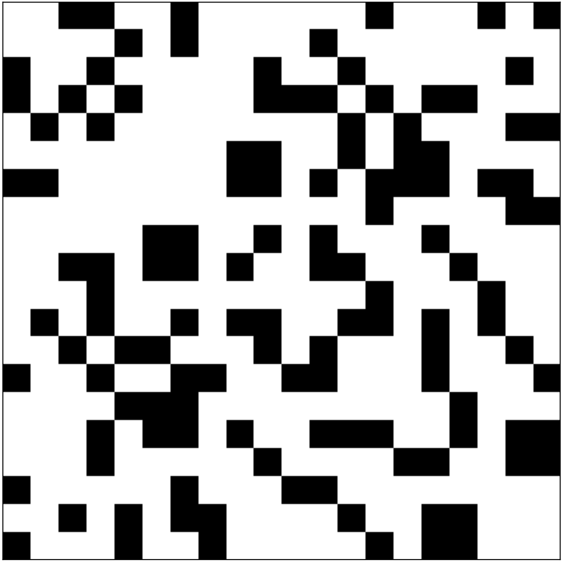
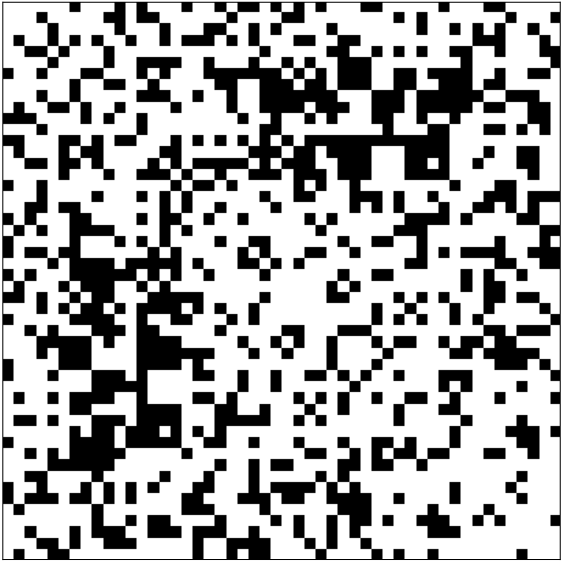
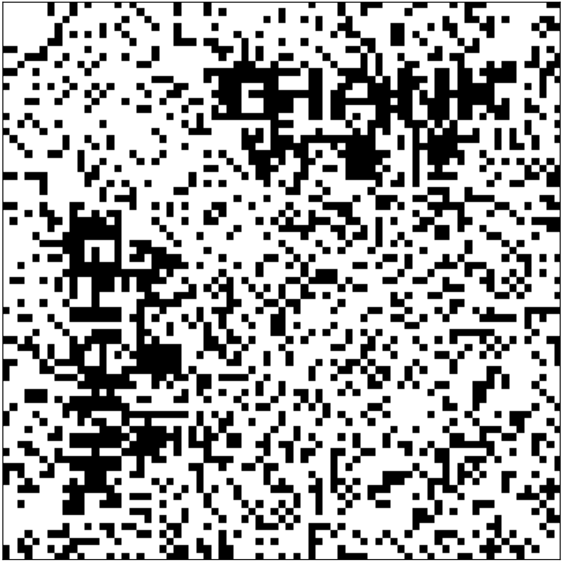
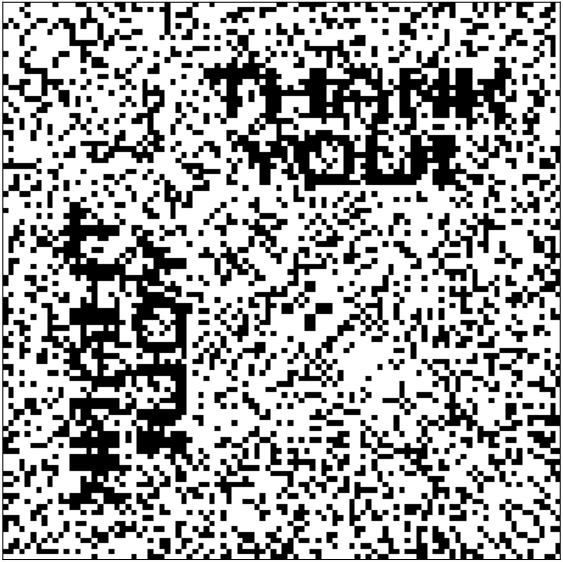
Answer: Convergence in merge distortion to graphon cluster tree.

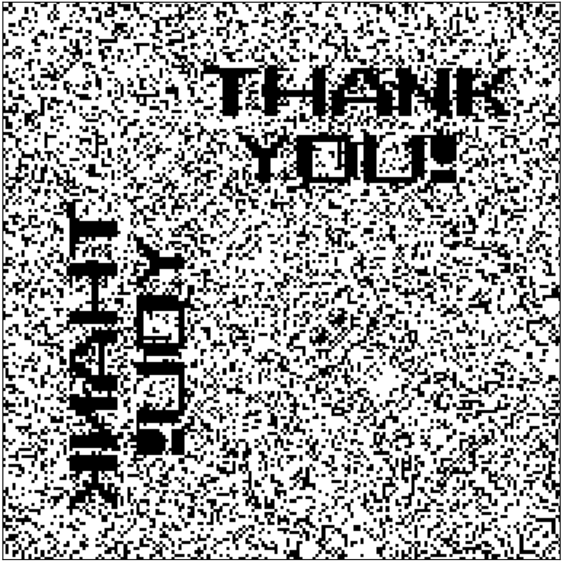
Question 3: How do we recover the correct clustering?
Answer: Modified neighborhood smoothing + single linkage clustering.










THANK YOU!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THANK YOU!

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Weak isomorphism

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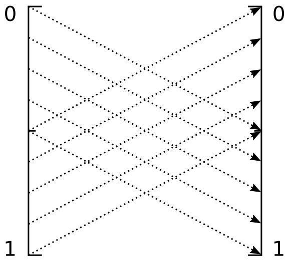
$$\varphi(x) = \begin{cases} x + 1/2 & x \leq 1/2, \\ x - 1/2 & x > 1/2 \end{cases}$$



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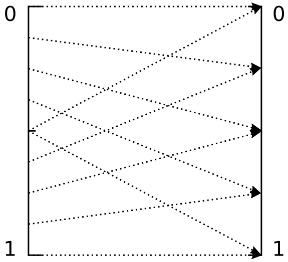
Notation: $W^{\varphi}(x,y) = W(\varphi(x), \varphi(y))$.

$$\varphi(x) = 2x \mod 1$$



Weak isomorphism

Definition (Lovász)

Two graphons W_1 and W_2 are weakly isomorphic if there exist measure preserving transformations φ_1 and φ_2 such that $W_1^{\varphi_1} \overset{\text{a.e.}}{=} W_2^{\varphi_2}$.

- W_1 and W_2 define the same distribution iff they are weakly isomorphic.

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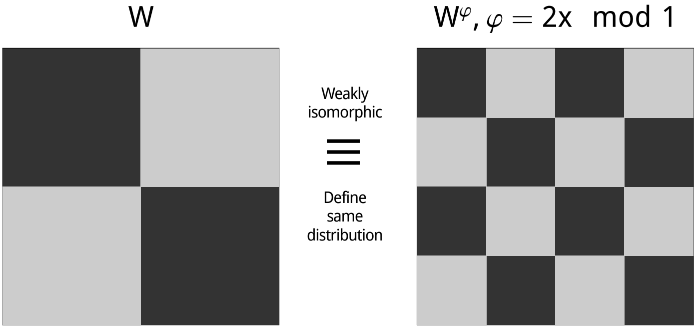


The clusters of a graphon

1. Collect all subsets of $[0, 1]$ which should be clustered at λ:

$$\mathfrak{A}_\lambda = \{A \subset [0,1] : \mu(A) > 0 \text{ and A is connected } \forall\, \lambda' < \lambda.\}$$

2. If $A_1, A_2, A \in \mathfrak{A}_\lambda$, and $A_1 \cup A_2 \subset A$, then A_1, A_2, and A should all be in the same cluster at λ. Consider them equivalent.
   - Define equivalence relation on $\mathfrak{A}_\lambda$:

$$A_1 \multimap\!\!\circ_\lambda A_2 \iff \exists A \in \mathfrak{A}_\lambda, A \supset A_1 \cup A_2.$$

   - Read: A_1 is clustered with A_2 at level λ.
   - $\multimap\!\!\circ_\lambda$ partitions $\mathfrak{A}_\lambda$ into equivalence classes of sets which should be in the same cluster.

The clusters of a graphon

3. Define clusters to be "largest" element of each equivalence class.
   - Subtlety in defining "largest":
     - Suppose $\mathscr{A} \in \mathfrak{A}_\lambda / \multimap_\lambda$ is such an equivalence class.
     - Let A be any representative from $\mathscr{A}$, let Z be a set of zero measure.
     - $A' = A \cup Z$ is a representative of $\mathscr{A}$.
   - In general there is no representative of $\mathscr{A}$ which strictly contains all other representatives in $\mathscr{A}$
   - We can find reps. which contain every other rep. up to a null set, called the "essential maxima" of $\mathscr{A}$:

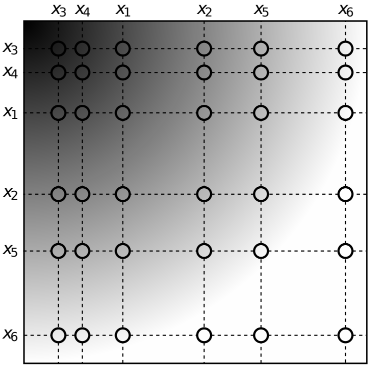
$$\operatorname{ess\,max} \mathscr{A} = \{A \in \mathscr{A} : \forall A' \in \mathscr{A}, \mu(A' \setminus A) = 0\}$$

   - The clusters of W at level λ are the essential maxima of each equivalence class:

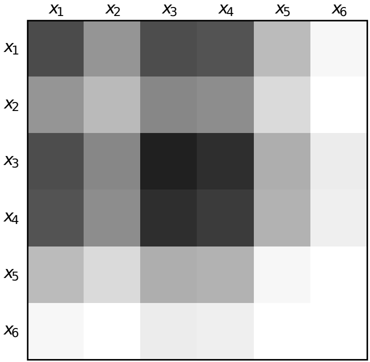
$$\mathbb{C}_W(\lambda) = \{\operatorname{ess\,max} \mathscr{A} : \mathscr{A} \in \mathfrak{A}_\lambda / \multimap_\lambda.\}$$

Consistent algorithms

- Intuitively, estimating the graphon is related to clustering.
- It suffices to estimate the so-called edge probability matrix.



W



$P : P_{ij} = W(x_i, x_j)$

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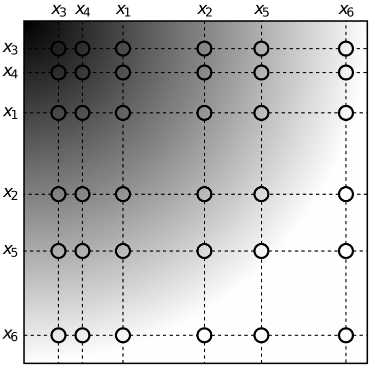

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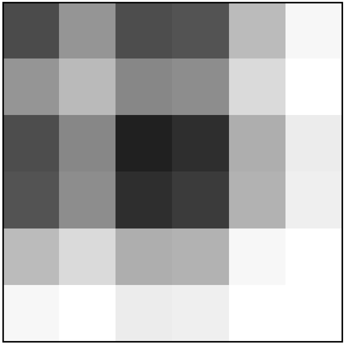

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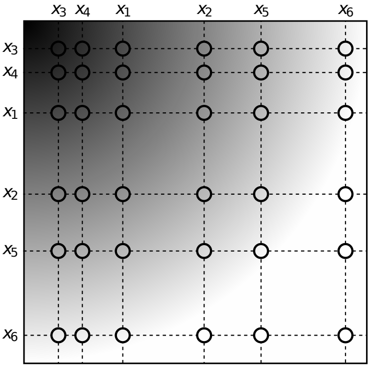

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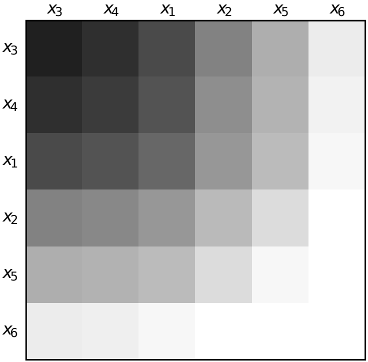
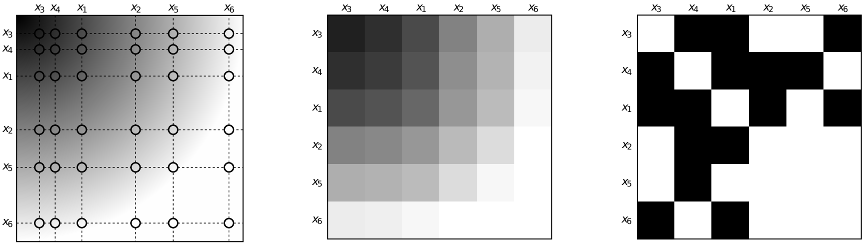


P (artificially permuted)

Sample an adjacency matrix A from P:



W

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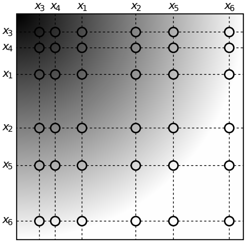
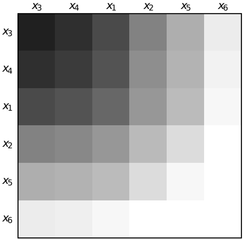


W



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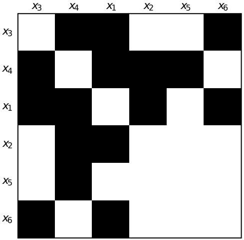
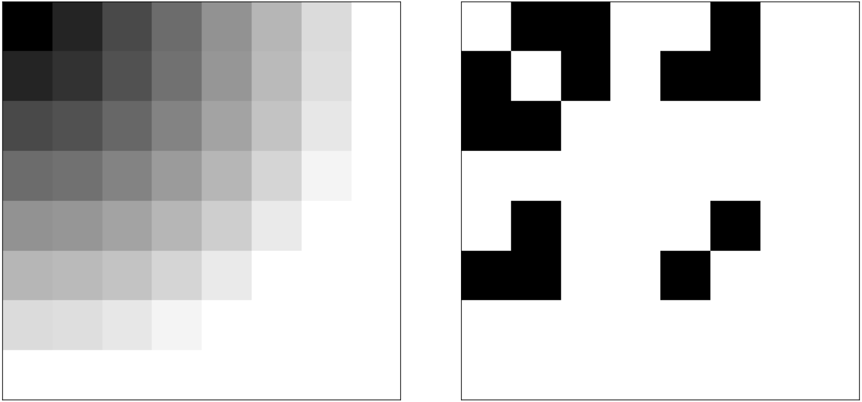


A

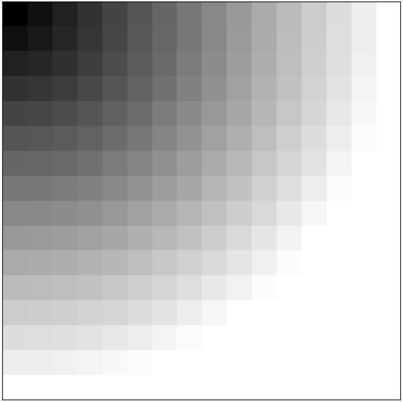
A is a poor estimate of P.

$$n = 8$$

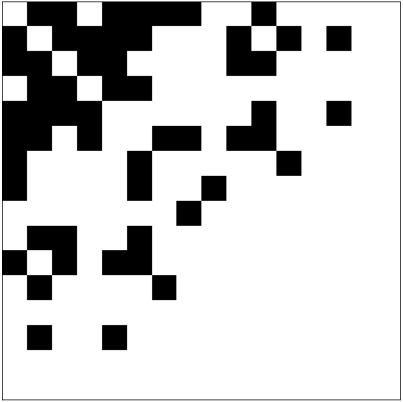


P A

$n = 16$

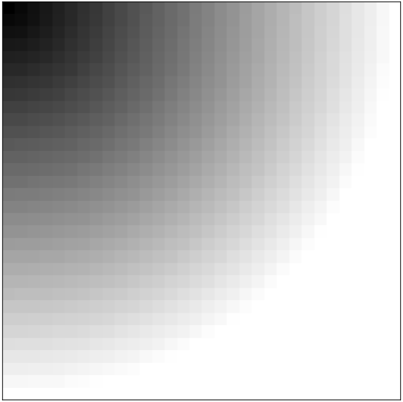


P

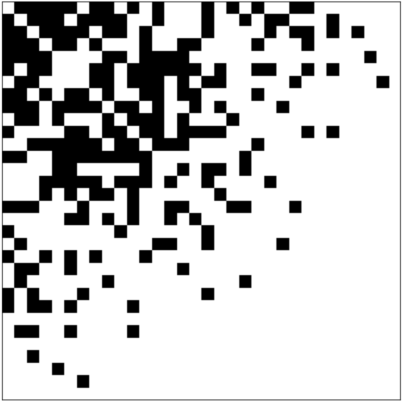


A

$n = 32$

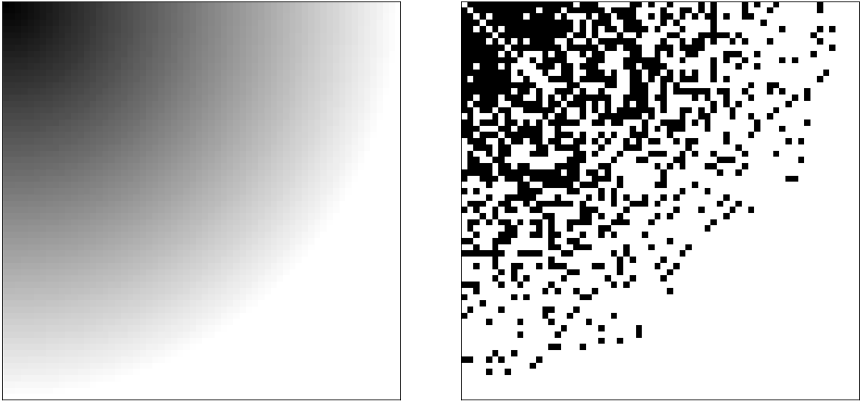


P



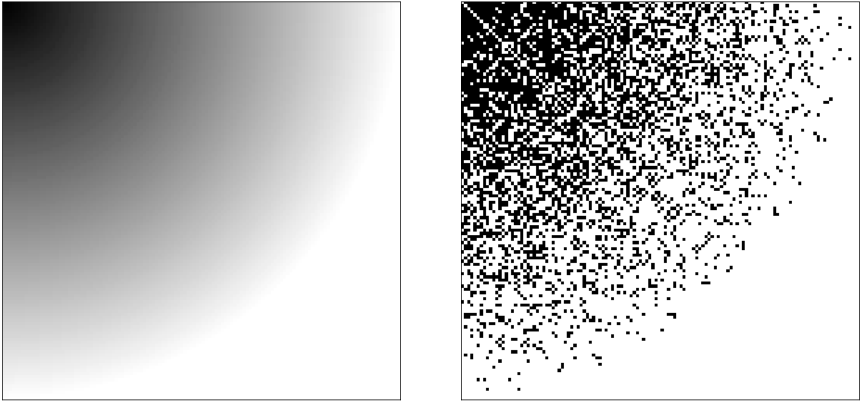
A

n = 64



P A

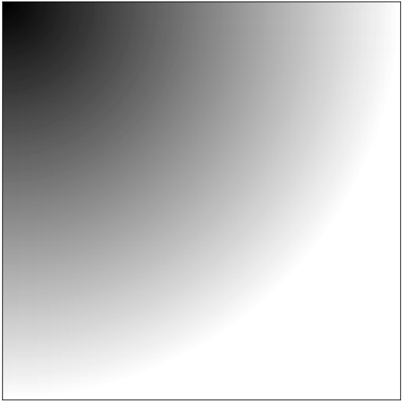
$n = 128$



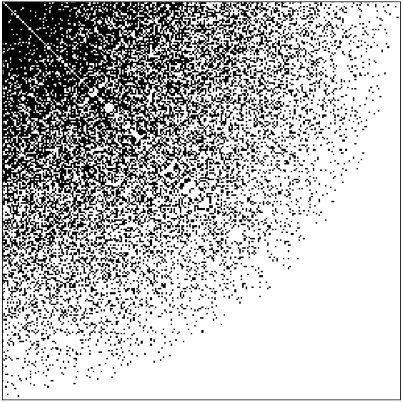
P

A

$n = 256$



P

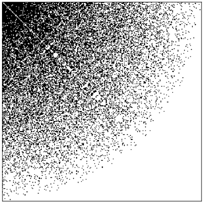


A

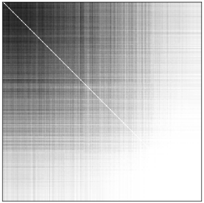
Edge probability estimation

Goal: Compute estimated edge probabilities $\hat{P}$ from A.

P



A



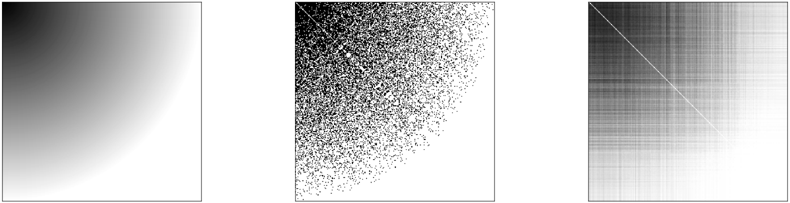
$\hat{P}$

Theorem

If $\|P - \hat{P}\|_\infty \to 0$ in probability as $n \to \infty$, then single linkage clustering on $\hat{P}$ is a consistent clustering method.

Edge probability estimation

Goal: Compute estimated edge probabilities $\hat{P}$ from A.



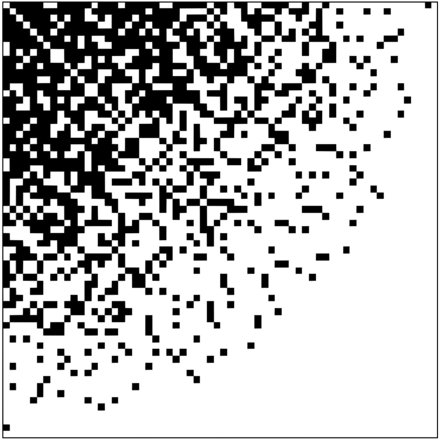
P $\qquad$ A $\qquad$ $\hat{P}$

Theorem

If $\|P - \hat{P}\|_\infty \to 0$ in probability as $n \to \infty$, then single linkage clustering on $\hat{P}$ is a consistent clustering method.

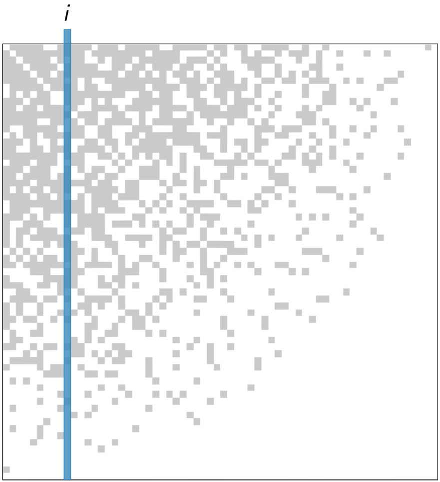
- We need a suitable estimator $\hat{P}$ of edge probabilities.
- Recently, Zhang et al. (2015) proposed neighborhood smoothing.

Neighborhood smoothing



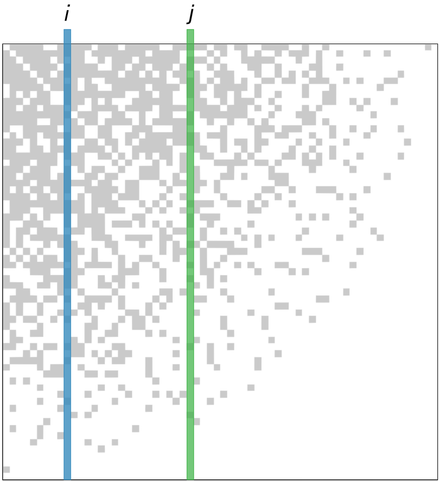
Given A, the adjacency matrix of a sampled graph...

Neighborhood smoothing



Consider a node i and its corresponding column of A.

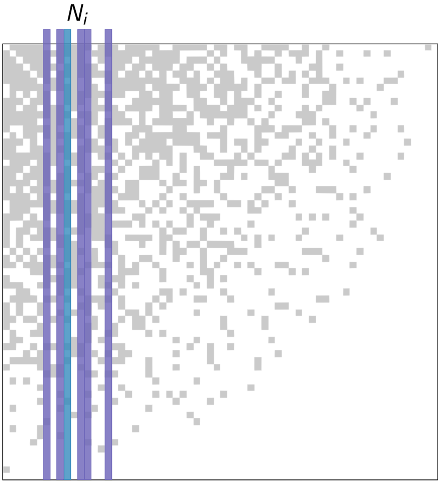
Neighborhood smoothing



Measure similarity to every other node j:

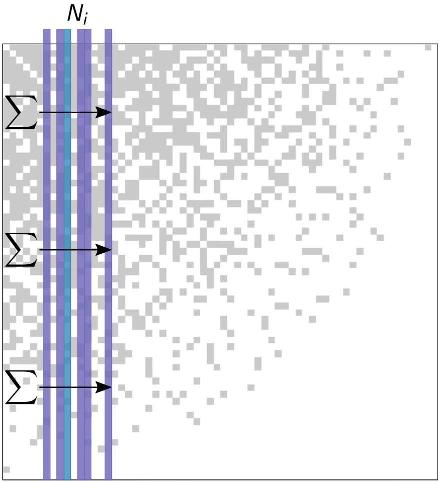
$$d(i,j) = \max_{k \neq i,j} \left| (A^2)_{ik} - (A^2)_{jk} \right|$$

Neighborhood smoothing



Form neighborhood N_i of nodes most similar to i.

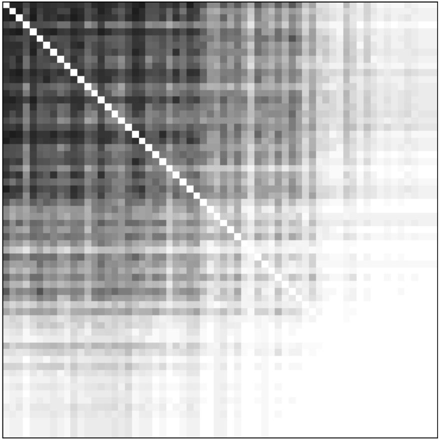
Neighborhood smoothing



Average within neighborhood to estimate edge probability:

$$\hat{P}_{ij} = \frac{1}{2|N_i|} \sum_{i' \in N_i} A_{i'j} + \frac{1}{2|N_j|} \sum_{j' \in N_j} A_{ij'}$$

Neighborhood smoothing



The result is a smoothed estimate $\hat{P}$ of edge probabilities.