priors on exchangeable directed graphs

Diana Cai

Department of Statistics University of Chicago

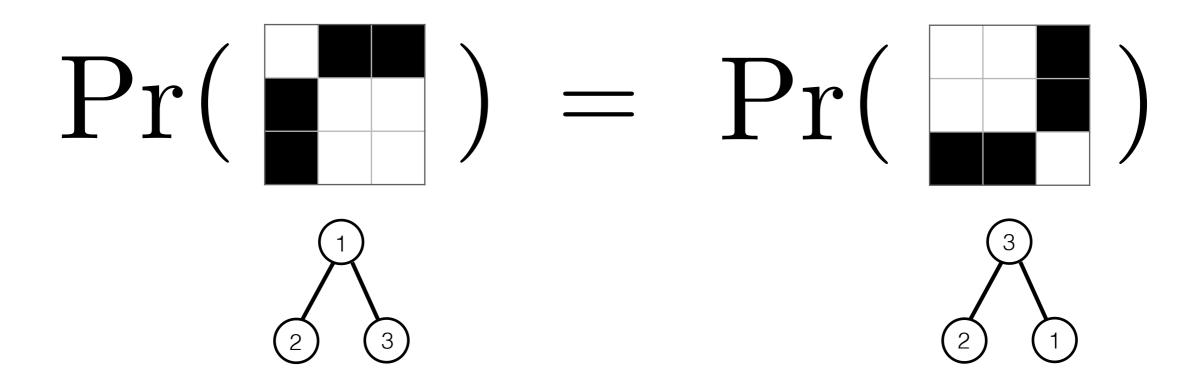
Collaborators:
Nathanael Ackerman (Harvard)
Cameron Freer (Gamalon and MIT)

Overview

- We consider exchangeable (dense) graphs.
- Specifically, we are interested in **directed** graphs.
 However, most work has focused on undirected graphs.
- Aldous-Hoover has an analogous statement for directed graphs, which is more complicated than merely using an asymmetric function.
- Many natural nonparametric priors on exchangeable undirected graphs extend to the directed case.
- This perspective leads to natural priors on other exchangeable structures, such as tournaments and directed acyclic graphs.

exchangeability:

order of vertices doesn't affect distribution of graph



Undirected Directed

Any exchangeable random infinite graph is obtained as a mixture of $\mathbb{G}(\infty, W)$.

 $\mathbb{G}(\infty,W)$ is a sampling procedure from the **graphon** W.

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

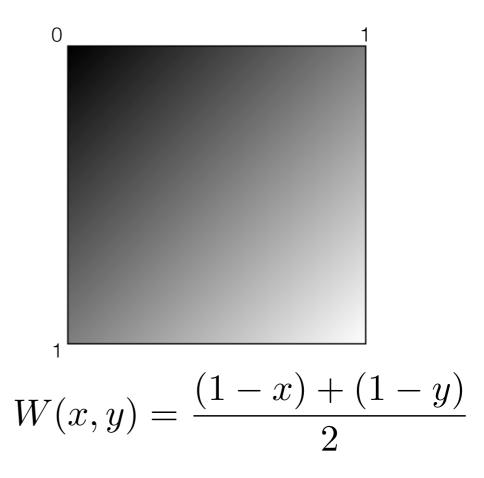
$$W(x,y) = W(y,x)$$

Aldous-Hoover

Graphon:

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

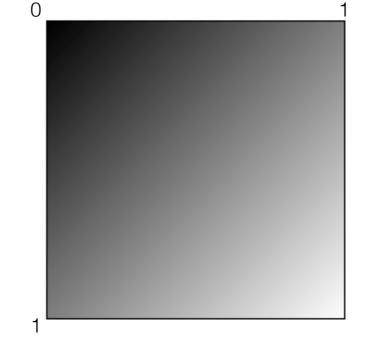
 $W(x,y) = W(y,x)$



Graphon:

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

 $W(x,y) = W(y,x)$



Sampling procedure:

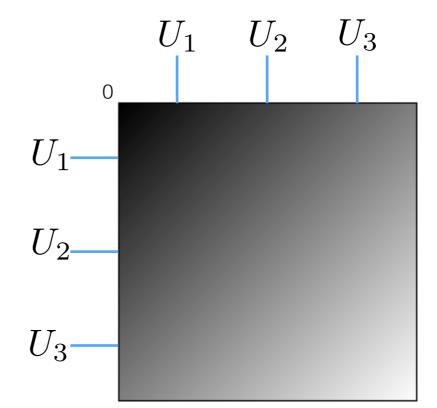
$$U_i \sim \text{Uniform}[0,1]$$

$$G_{ij} \sim \text{Bern}(W(U_i, U_j)), i < j \quad (\text{Set } G_{ji} = G_{ij})$$

Graphon:

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

 $W(x,y) = W(y,x)$



Sampling procedure:

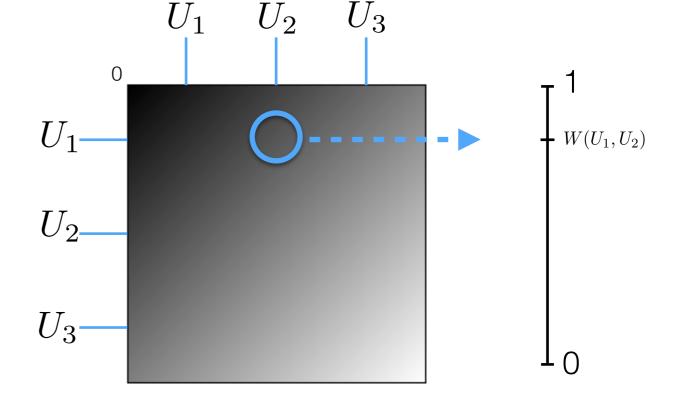
$$U_i \sim \text{Uniform}[0,1]$$

$$G_{ij} \sim \text{Bern}(W(U_i, U_j)), i < j \quad (\text{Set } G_{ji} = G_{ij})$$

Graphon:

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

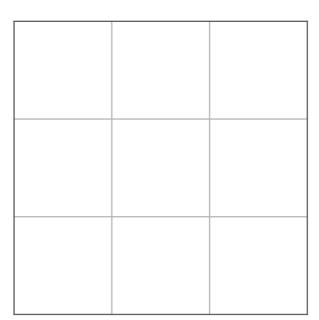
 $W(x,y) = W(y,x)$



Sampling procedure:

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

$$G_{ij} \sim \text{Bern}(W(U_i, U_j)), i < j$$



Graphon:

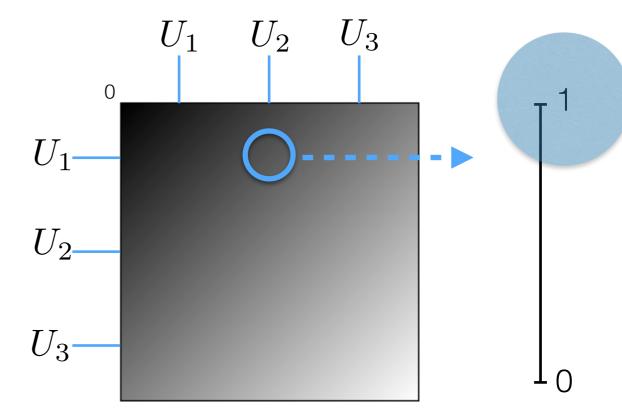
$$W: [0,1]^2 \to [0,1]$$

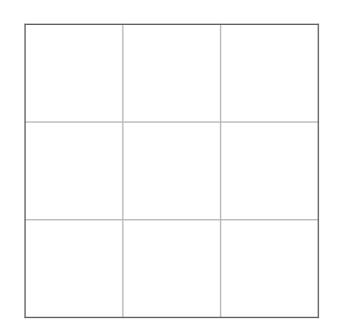
 $W(x,y) = W(y,x)$



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

$$G_{ij} \sim \text{Bern}(W(U_i, U_j)), i < j$$





Graphon:

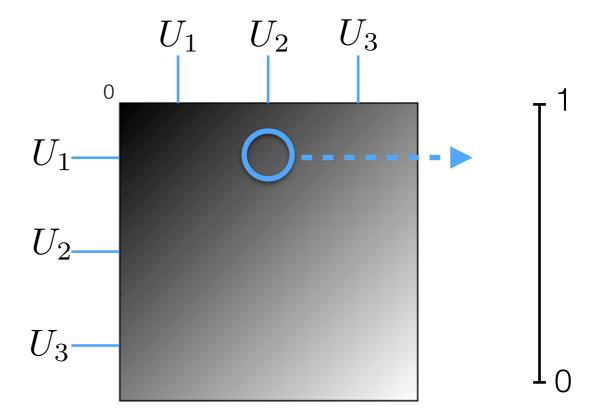
$$W: [0,1]^2 \to [0,1]$$

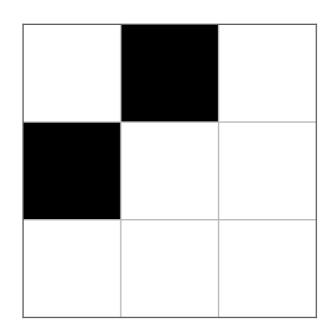
 $W(x,y) = W(y,x)$



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

$$G_{ij} \sim \text{Bern}(W(U_i, U_j)), i < j$$





Many results for exchangeable **undirected** graphs extend to **directed** graphs.

Many results for exchangeable **undirected** graphs extend to **directed** graphs.

order of vertices doesn't affect distribution of graph

$$\Pr(\square) = \Pr(\square)$$

Undirected

Directed

Any exchangeable random infinite graph is obtained as a mixture of $\mathbb{G}(\infty, W)$.

 $\mathbb{G}(\infty,W)$ is a sampling procedure from the **graphon** W.

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

$$W(x,y) = W(y,x)$$

Any exchangeable random infinite **digraph** is obtained as a mixture of $\mathbb{G}(\infty, \mathbf{W})$.

 $\mathbb{G}(\infty, \boldsymbol{W})$ is a sampling procedure from the **digraphon** \boldsymbol{W} .

$$W = ?$$

Aldous-Hoover; cf. Lovász-Szegedy implicit in A–H; cf. Diaconis–Janson

Can we just use a single **asymmetric** measurable function?

Can we just use a single **asymmetric** measurable function?

Yes, by independently choosing each edge direction.

Can we just use a single **asymmetric** measurable function?

Yes, by independently choosing each edge direction.

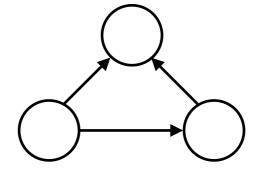
But this does not cover *all* directed graphs:

Can we just use a single **asymmetric** measurable function?

Yes, by independently choosing each edge direction.

But this does not cover all directed graphs:

• tournaments (each pair of vertices has exactly one directed edge)

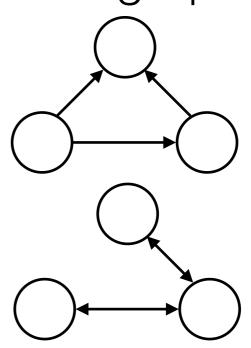


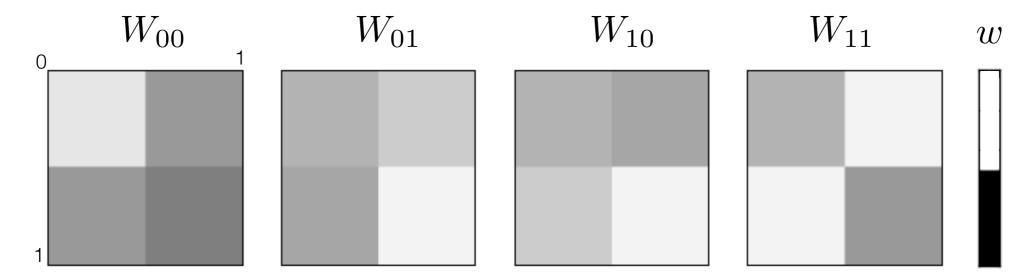
Can we just use a single **asymmetric** measurable function?

Yes, by independently choosing each edge direction.

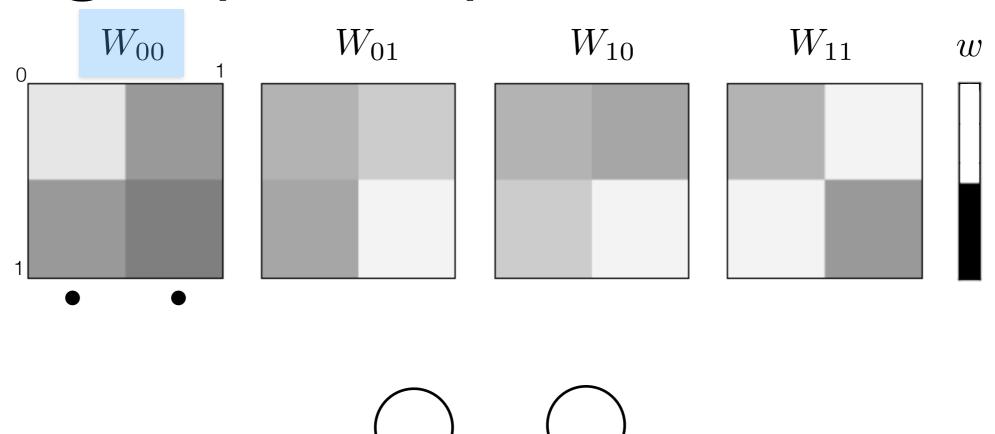
But this does not cover all directed graphs:

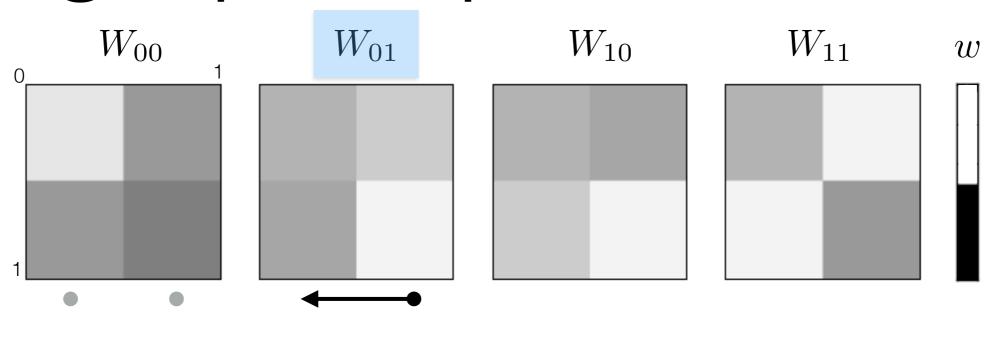
- tournaments (each pair of vertices has exactly one directed edge)
- undirected graphs (each pair has either both or no directed edges)

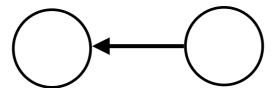


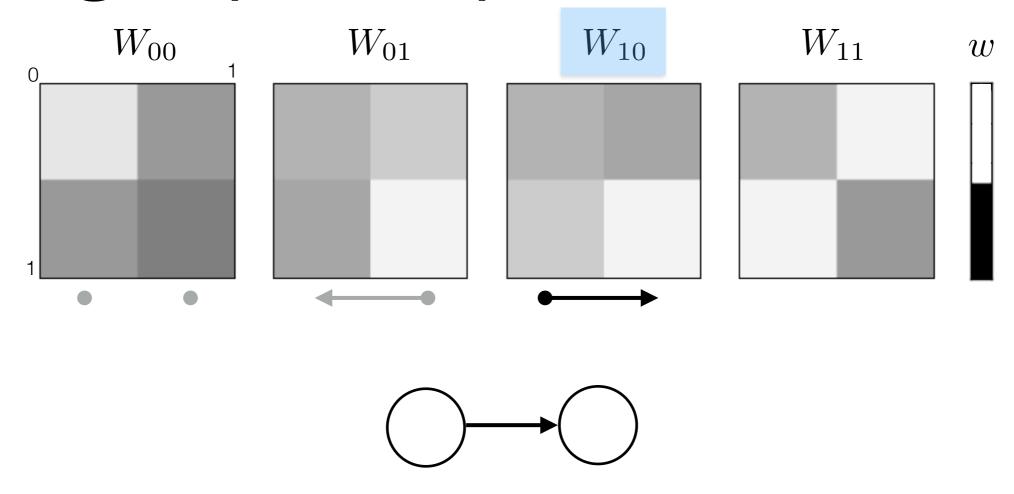


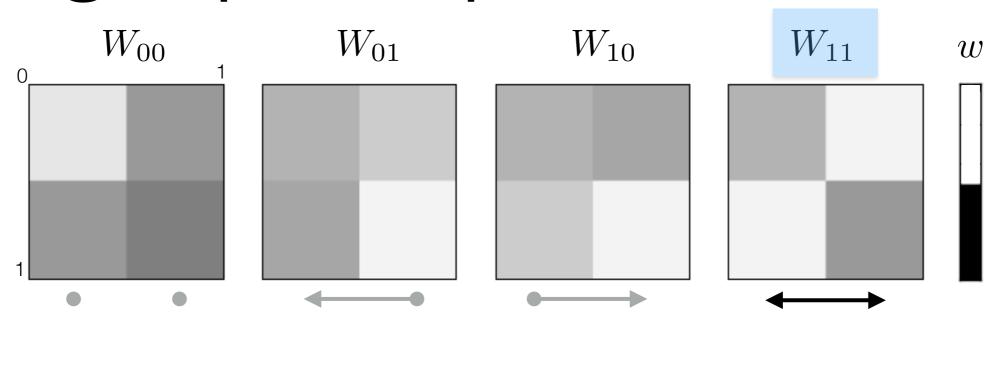
- Digraphon: $\mathbf{W} = (W_{00}, W_{01}, W_{10}, W_{11}, w)$
 - $W_{ab}:[0,1]^2 \rightarrow [0,1]$ and $w:[0,1] \rightarrow \{0,1\}$ measurable functions
- For $a, b \in \{0, 1\}$ and $x, y \in [0, 1]$,
 - 1. $W_{ab}(x,y) = W_{ba}(y,x)$, when a = b
 - 2. $W_{ab}(x,y) = W_{ba}(y,x)$, when $a \neq b$
 - 3. $\sum_{a,b} W_{a,b}(x,y) = 1$

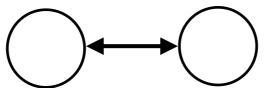


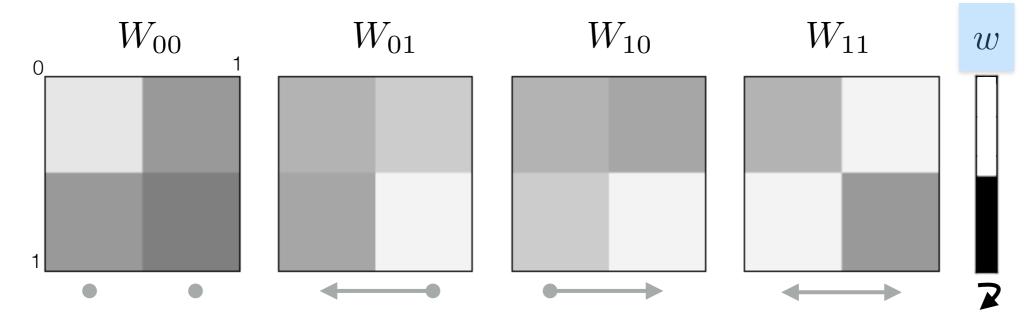




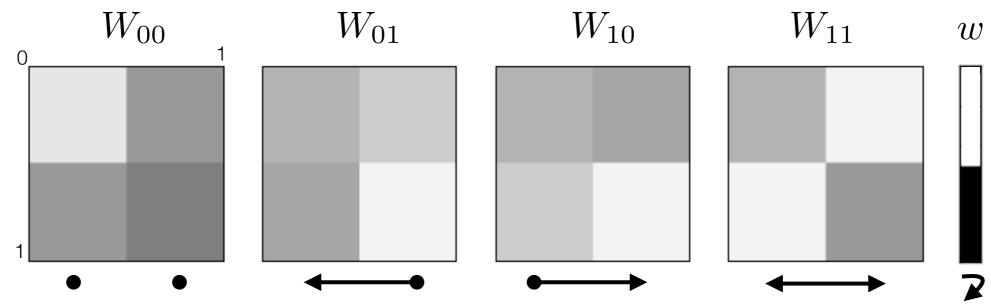






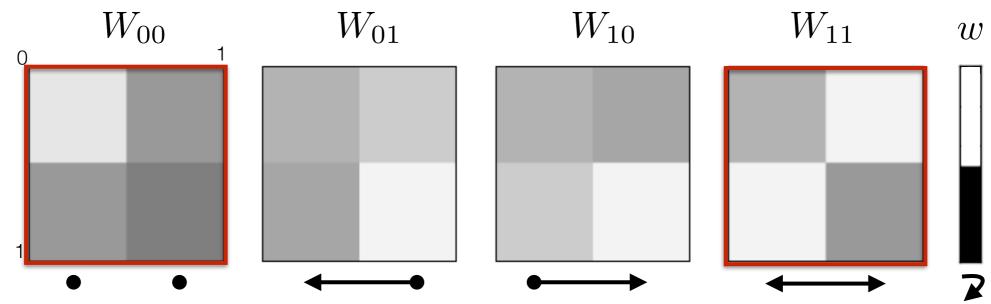






- Digraphon: $\mathbf{W} = (W_{00}, W_{01}, W_{10}, W_{11}, w)$
 - $W_{ab}:[0,1]^2 \rightarrow [0,1]$ and $w:[0,1] \rightarrow \{0,1\}$ measurable functions
- For $a, b \in \{0, 1\}$ and $x, y \in [0, 1]$,
 - 1. $W_{ab}(x,y) = W_{ba}(y,x)$, when a = b
 - 2. $W_{ab}(x,y) = W_{ba}(y,x)$, when $a \neq b$

3.
$$\sum_{a,b} W_{a,b}(x,y) = 1$$

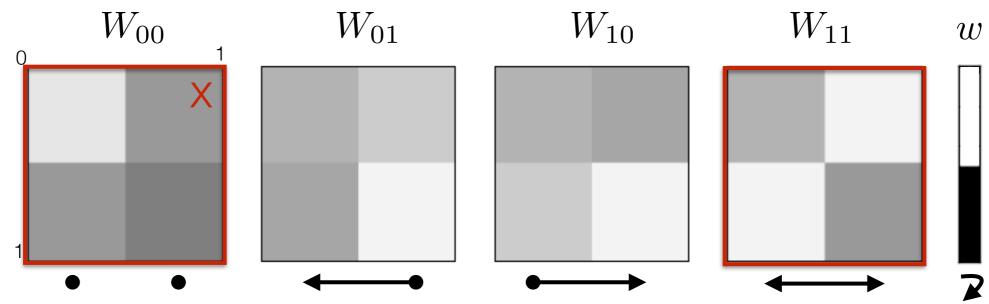


- Digraphon: $\mathbf{W} = (W_{00}, W_{01}, W_{10}, W_{11}, w)$
 - $W_{ab}:[0,1]^2 \rightarrow [0,1]$ and $w:[0,1] \rightarrow \{0,1\}$ measurable functions
- For $a, b \in \{0, 1\}$ and $x, y \in [0, 1]$,

1.
$$W_{ab}(x,y) = W_{ba}(y,x)$$
, when $a = b$

2.
$$W_{ab}(x,y) = W_{ba}(y,x)$$
, when $a \neq b$

3.
$$\sum_{a,b} W_{a,b}(x,y) = 1$$

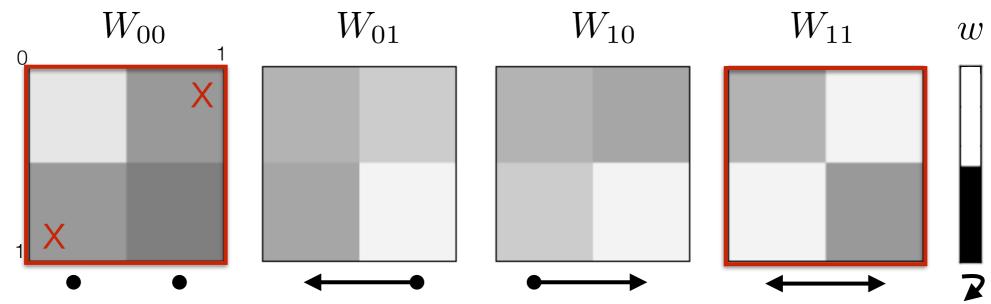


- Digraphon: $\mathbf{W} = (W_{00}, W_{01}, W_{10}, W_{11}, w)$
 - $W_{ab}:[0,1]^2 \rightarrow [0,1]$ and $w:[0,1] \rightarrow \{0,1\}$ measurable functions
- For $a, b \in \{0, 1\}$ and $x, y \in [0, 1]$,

1.
$$W_{ab}(x,y) = W_{ba}(y,x)$$
, when $a = b$

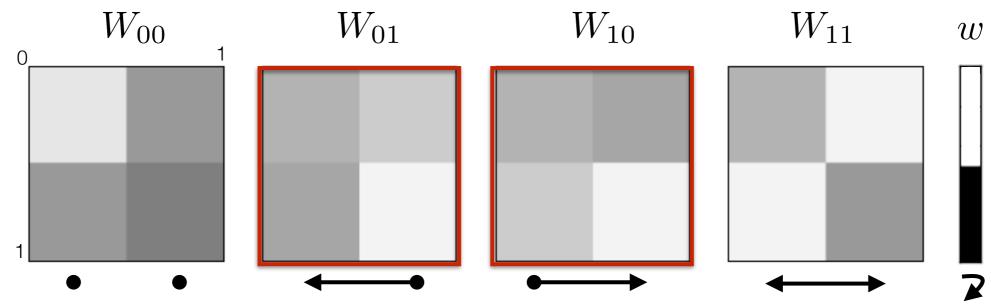
2.
$$W_{ab}(x,y) = W_{ba}(y,x)$$
, when $a \neq b$

3.
$$\sum_{a,b} W_{a,b}(x,y) = 1$$



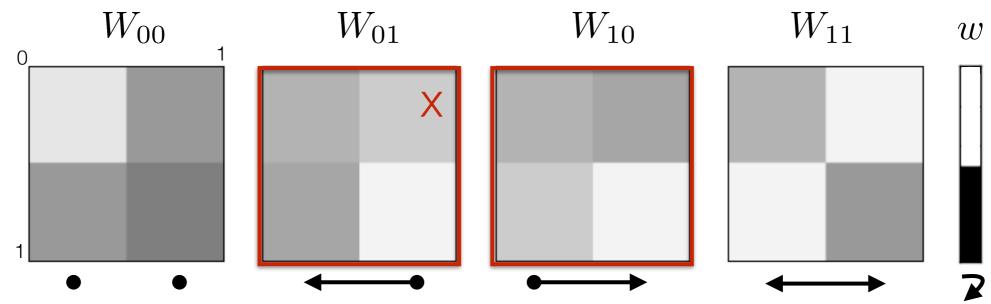
- Digraphon: $\mathbf{W} = (W_{00}, W_{01}, W_{10}, W_{11}, w)$
 - $W_{ab}:[0,1]^2 \rightarrow [0,1]$ and $w:[0,1] \rightarrow \{0,1\}$ measurable functions
- For $a, b \in \{0, 1\}$ and $x, y \in [0, 1]$,
 - 1. $W_{ab}(x,y) = W_{ba}(y,x)$, when a = b
 - 2. $W_{ab}(x,y) = W_{ba}(y,x)$, when $a \neq b$

3.
$$\sum_{a,b} W_{a,b}(x,y) = 1$$



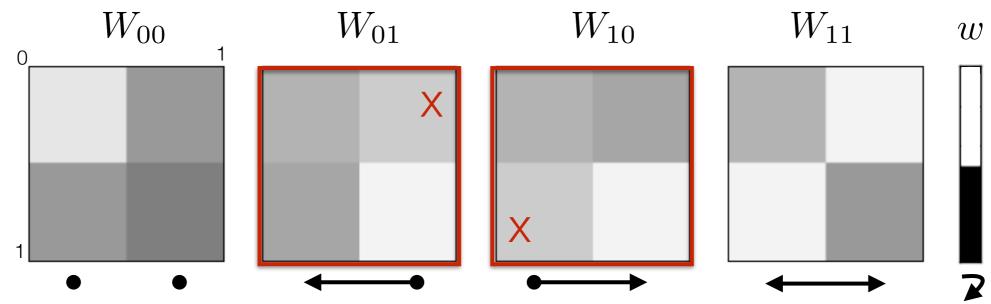
- Digraphon: $\mathbf{W} = (W_{00}, W_{01}, W_{10}, W_{11}, w)$
 - $W_{ab}:[0,1]^2 \rightarrow [0,1]$ and $w:[0,1] \rightarrow \{0,1\}$ measurable functions
- For $a, b \in \{0, 1\}$ and $x, y \in [0, 1]$,
 - 1. $W_{ab}(x,y) = W_{ba}(y,x)$, when a = b
 - 2. $W_{ab}(x,y) = W_{ba}(y,x)$, when $a \neq b$

3.
$$\sum_{a,b} W_{a,b}(x,y) = 1$$



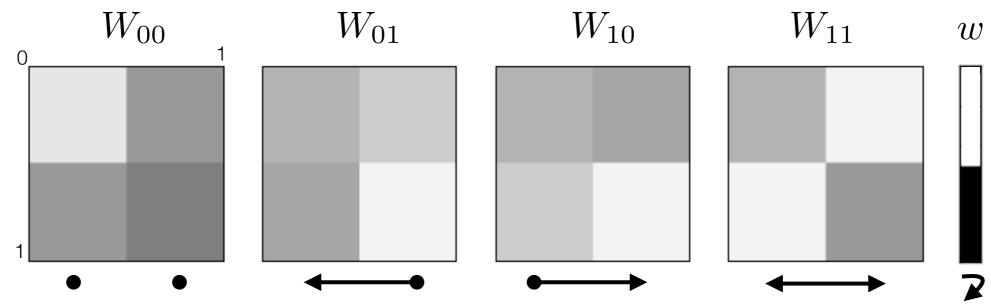
- Digraphon: $\mathbf{W} = (W_{00}, W_{01}, W_{10}, W_{11}, w)$
 - $W_{ab}:[0,1]^2 \rightarrow [0,1]$ and $w:[0,1] \rightarrow \{0,1\}$ measurable functions
- For $a, b \in \{0, 1\}$ and $x, y \in [0, 1]$,
 - 1. $W_{ab}(x,y) = W_{ba}(y,x)$, when a = b
 - 2. $W_{ab}(x,y) = W_{ba}(y,x)$, when $a \neq b$

3.
$$\sum_{a,b} W_{a,b}(x,y) = 1$$



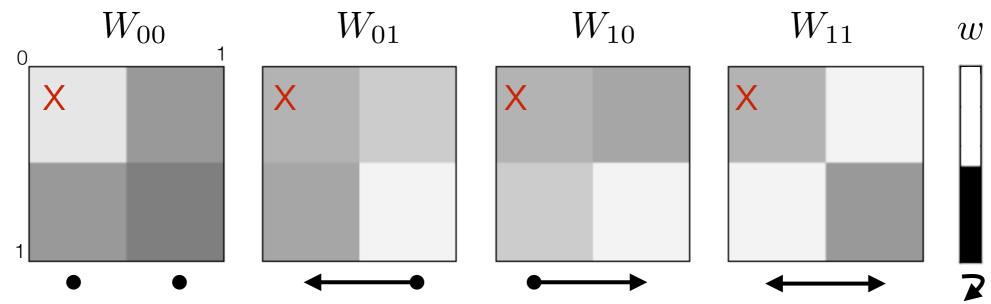
- Digraphon: $\mathbf{W} = (W_{00}, W_{01}, W_{10}, W_{11}, w)$
 - $W_{ab}:[0,1]^2 \rightarrow [0,1]$ and $w:[0,1] \rightarrow \{0,1\}$ measurable functions
- For $a, b \in \{0, 1\}$ and $x, y \in [0, 1]$,
 - 1. $W_{ab}(x,y) = W_{ba}(y,x)$, when a = b
 - 2. $W_{ab}(x,y) = W_{ba}(y,x)$, when $a \neq b$

3.
$$\sum_{a,b} W_{a,b}(x,y) = 1$$



- Digraphon: $\mathbf{W} = (W_{00}, W_{01}, W_{10}, W_{11}, w)$
 - $W_{ab}:[0,1]^2 \rightarrow [0,1]$ and $w:[0,1] \rightarrow \{0,1\}$ measurable functions
- For $a, b \in \{0, 1\}$ and $x, y \in [0, 1]$,
 - 1. $W_{ab}(x,y) = W_{ba}(y,x)$, when a = b
 - 2. $W_{ab}(x,y) = W_{ba}(y,x)$, when $a \neq b$

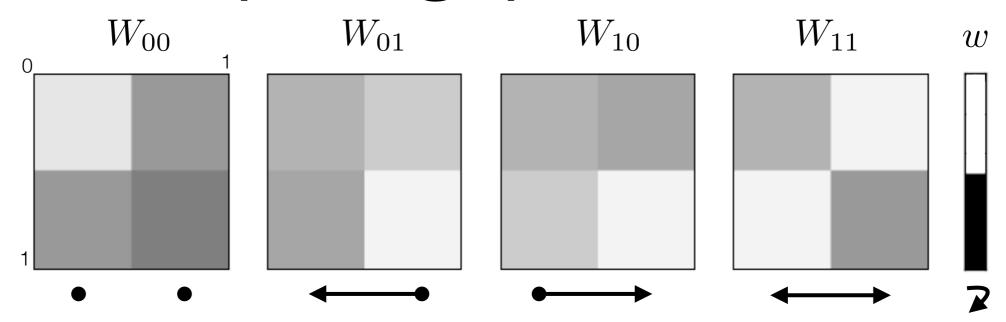
3.
$$\sum_{a,b} W_{a,b}(x,y) = 1$$



- Digraphon: $\mathbf{W} = (W_{00}, W_{01}, W_{10}, W_{11}, w)$
 - $W_{ab}:[0,1]^2 \rightarrow [0,1]$ and $w:[0,1] \rightarrow \{0,1\}$ measurable functions
- For $a, b \in \{0, 1\}$ and $x, y \in [0, 1]$,
 - 1. $W_{ab}(x,y) = W_{ba}(y,x)$, when a = b
 - 2. $W_{ab}(x,y) = W_{ba}(y,x)$, when $a \neq b$

3.
$$\sum_{a,b} W_{a,b}(x,y) = 1$$

Sampling procedure

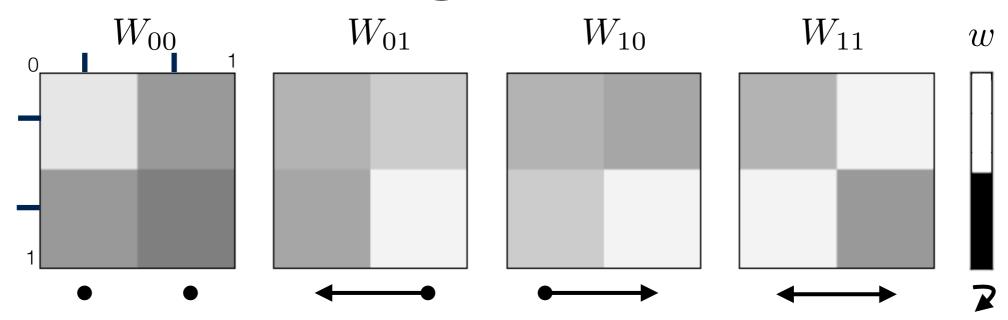


• Define $W_4(x,y) := (W_{00}(x,y), W_{01}(x,y), W_{10}(x,y), W_{11}(x,y))$

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

 $E_{ij} \sim \text{Categorical}(\boldsymbol{W}_4(U_i, U_j)), \text{ for } i < j$
 $G_{ij}, G_{ji} = \text{directed edge(s) corresponding to } E_{ij}, \text{ for } i < j$
 $G_{ii} = w(U_i)$

Sampling procedure



• Define $W_4(x,y) := (W_{00}(x,y), W_{01}(x,y), W_{10}(x,y), W_{11}(x,y))$

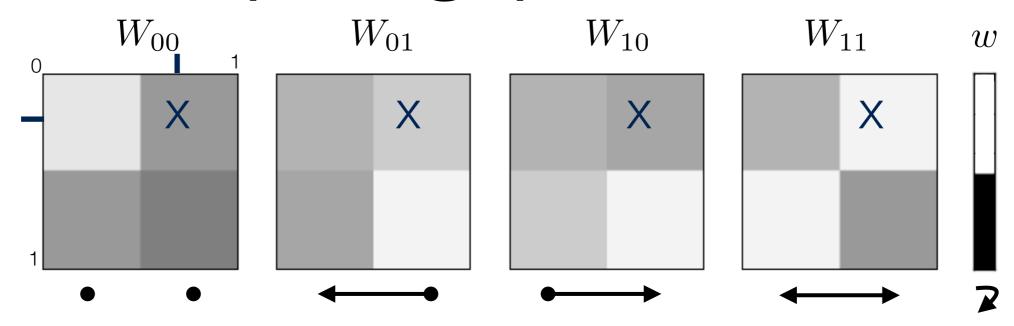
$U_i \sim \text{Uniform}[0,1]$

 $E_{ij} \sim \text{Categorical}(\boldsymbol{W}_4(U_i, U_j)), \text{ for } i < j$

 $G_{ij}, G_{ji} = \text{directed edge(s) corresponding to } E_{ij}, \text{ for } i < j$

$$G_{ii} = w(U_i)$$

Sampling procedure



• Define $W_4(x,y) := (W_{00}(x,y), W_{01}(x,y), W_{10}(x,y), W_{11}(x,y))$

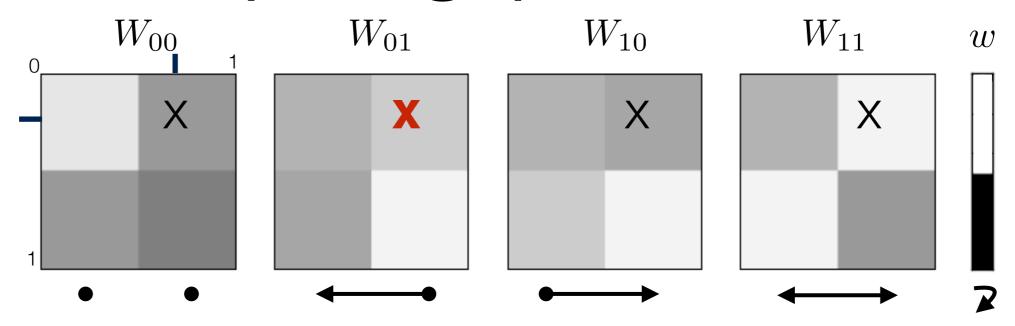
$$U_i \sim \text{Uniform}[0,1]$$

$$E_{ij} \sim \text{Categorical}(\boldsymbol{W}_4(U_i, U_j)), \text{ for } i < j$$

$$G_{ij}, G_{ji} = \text{directed edge(s) corresponding to } E_{ij}, \text{ for } i < j$$

$$G_{ii} = w(U_i)$$

Sampling procedure



• Define $W_4(x,y) := (W_{00}(x,y), W_{01}(x,y), W_{10}(x,y), W_{11}(x,y))$

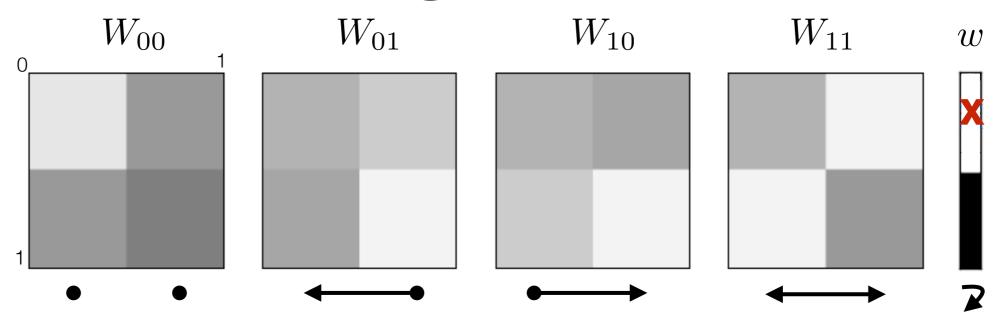
$$U_i \sim \text{Uniform}[0,1]$$

$$E_{ij} \sim \text{Categorical}(\boldsymbol{W}_4(U_i, U_j)), \text{ for } i < j$$

$$G_{ij}, G_{ji} = \text{directed edge(s) corresponding to } E_{ij}, \text{ for } i < j$$

$$G_{ii} = w(U_i)$$

Sampling procedure



• Define $W_4(x,y) := (W_{00}(x,y), W_{01}(x,y), W_{10}(x,y), W_{11}(x,y))$

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

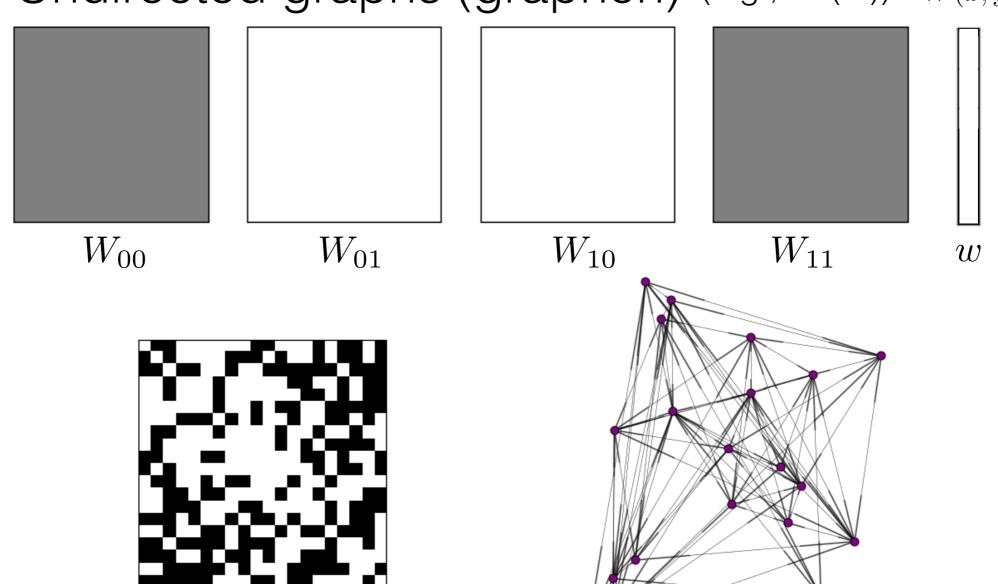
$$E_{ij} \sim \text{Categorical}(\boldsymbol{W}_4(U_i, U_j)), \text{ for } i < j$$

 $G_{ij}, G_{ji} = \text{directed edge(s) corresponding to } E_{ij}, \text{ for } i < j$

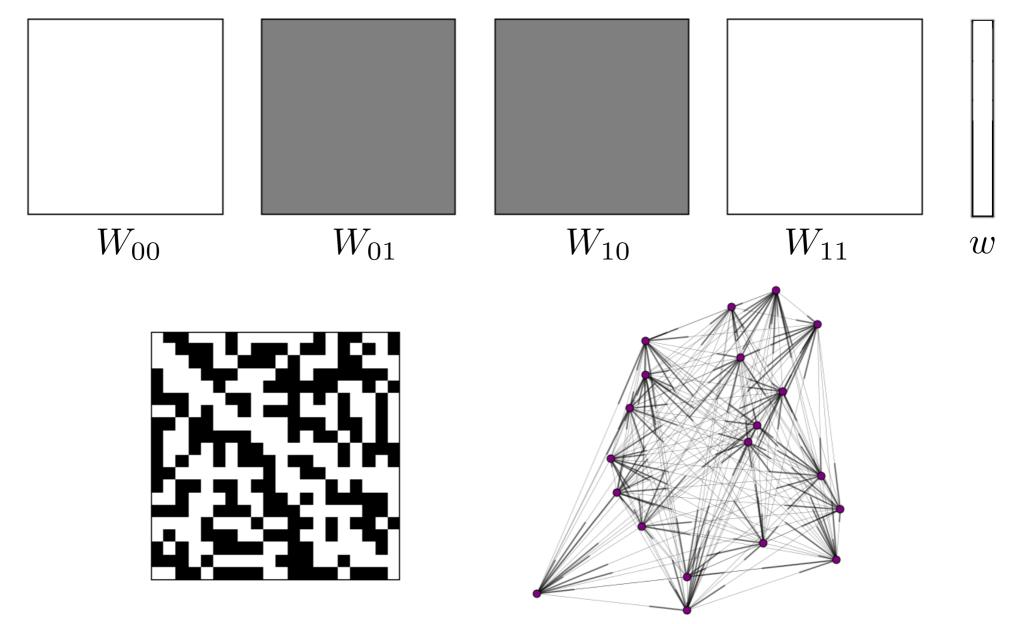
$$G_{ii} = w(U_i)$$

• Undirected graphs (graphon) (e.g., ER(½)) W(x,y) = W(y,x)

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

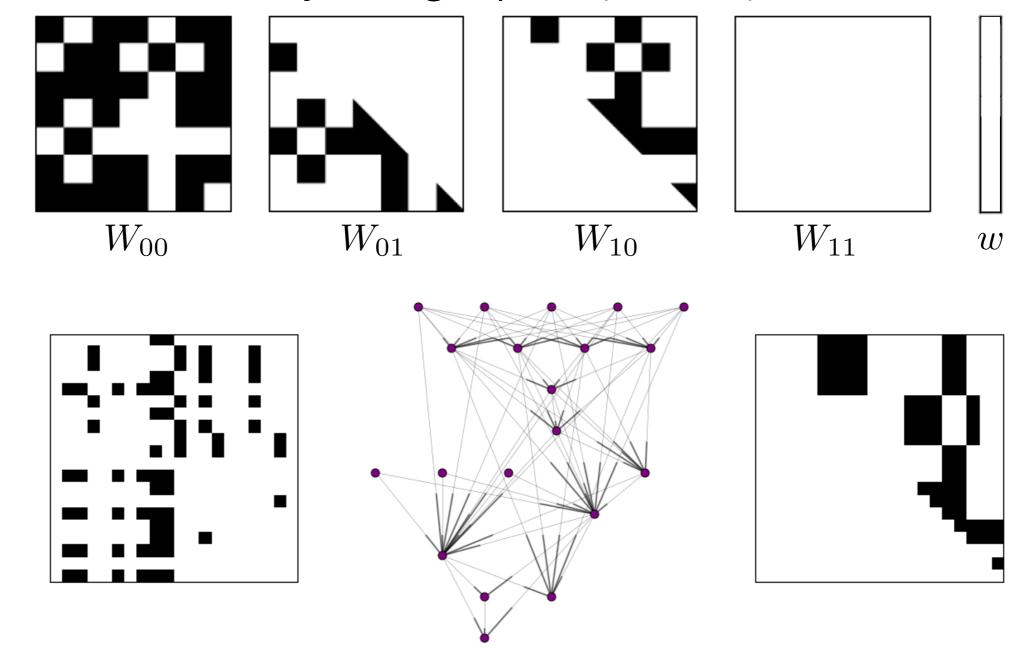


• Tournaments (e.g., generic tournament)

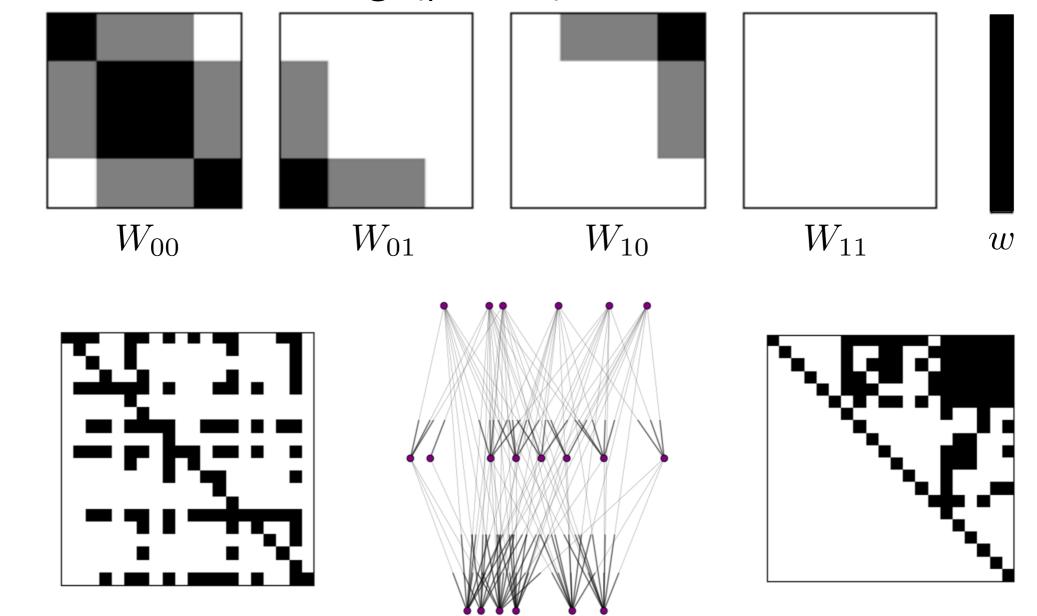


 Linear ordering (the only one, by Glasner-Weiss) W_{10} W_{00} W_{01} W_{11} w

Directed acyclic graphs (DAGs)

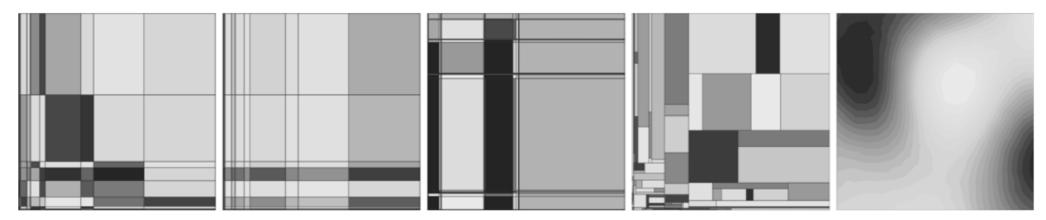


Partial ordering (poset)



Priors on digraphons

 Can extend literature for graphon priors (cf. Orbanz– Roy) to directed graphs, e.g., infinite relational model



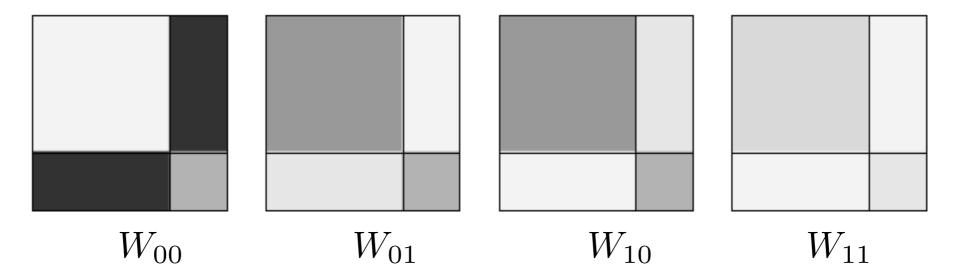
[Orbanz-Roy, 2015]

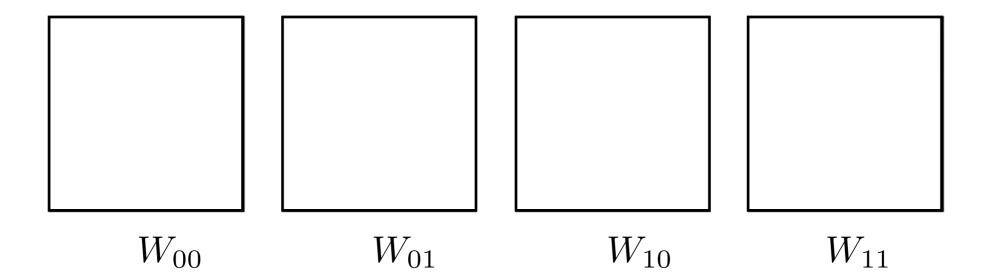
 Some of these models are already intended for directed graphs, via an asymmetric measurable function (to describe independent edge directions).

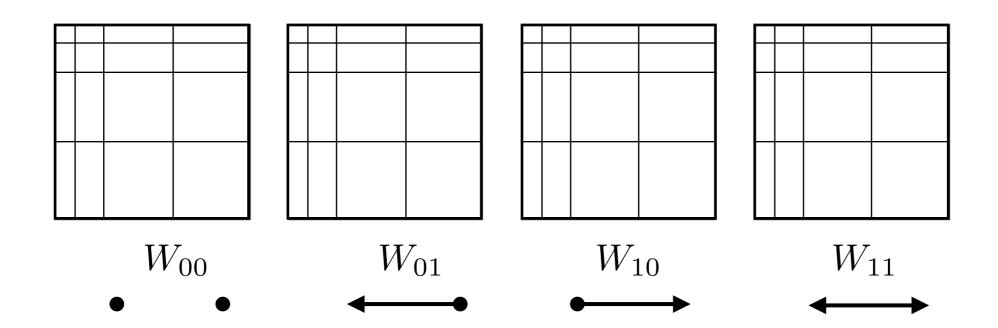
Directed block models

- In a block model, pairs of regions can vary in how tournament-like, as well as how dense they are:
 - e.g., Directed stochastic block model [Wang– Wong, 1987]

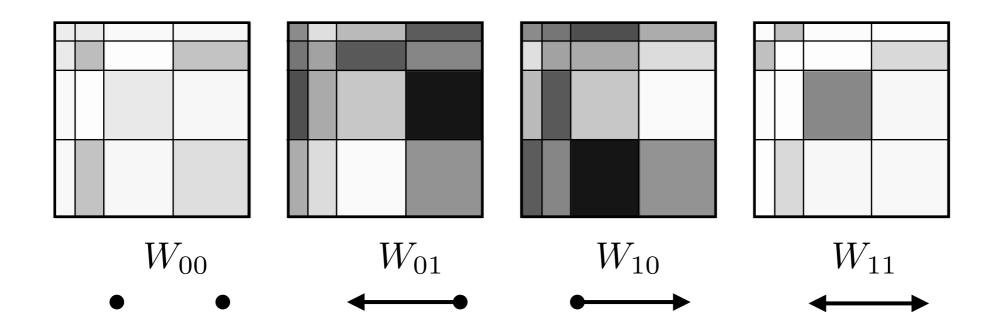
Example of SBM digraphon, 0.7 division



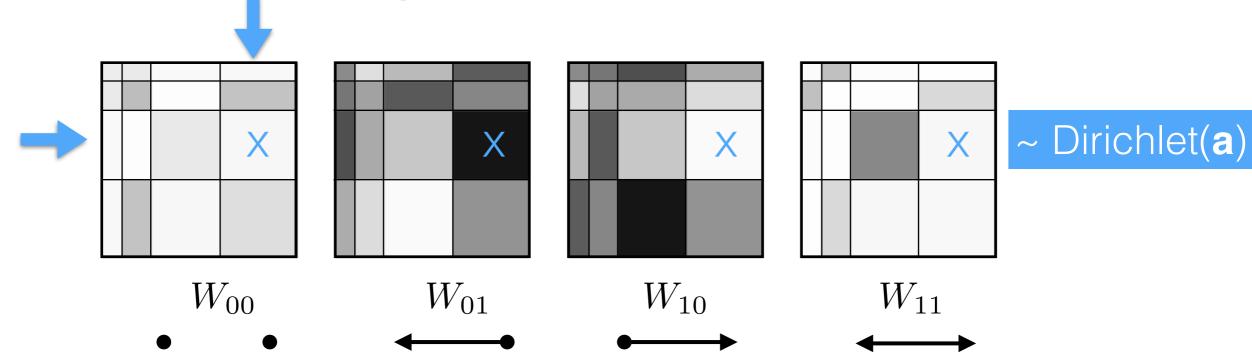




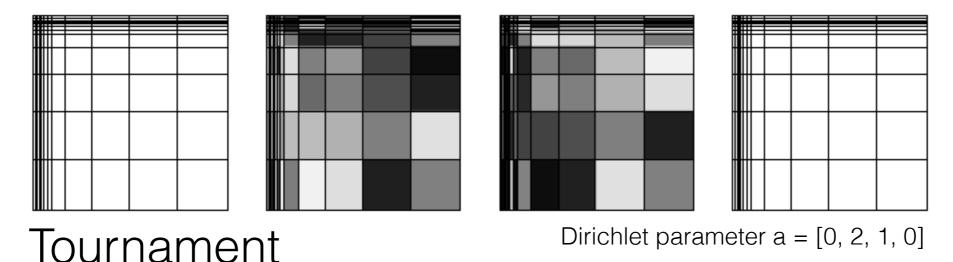
Draw partition ~ DP-Stick(alpha)

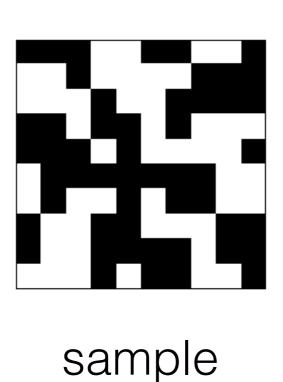


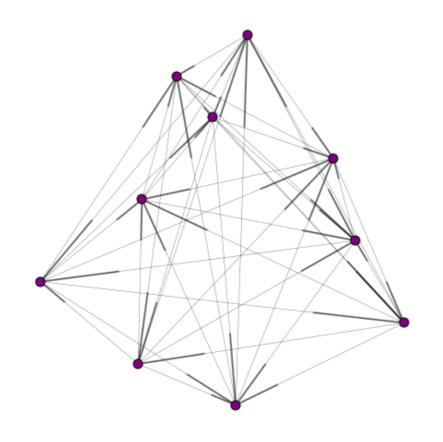
- Draw partition ~ DP-Stick(alpha)
- 2. Draw weights ~ Dirichlet(a)

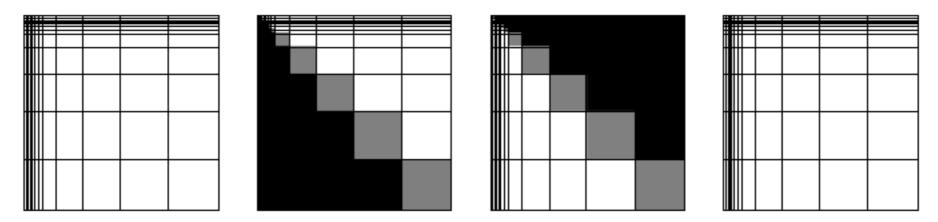


- 1. Draw partition ~ DP-Stick(alpha)
- 2. Draw weights ~ Dirichlet(a)



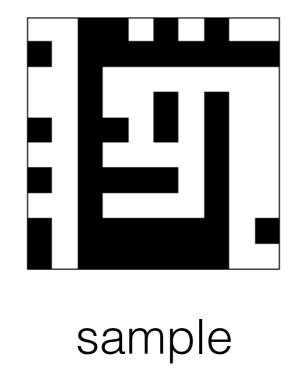


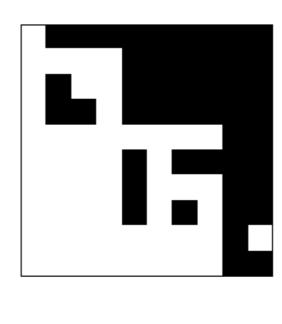


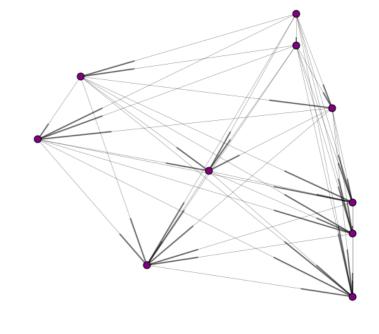


Almost totally ordered

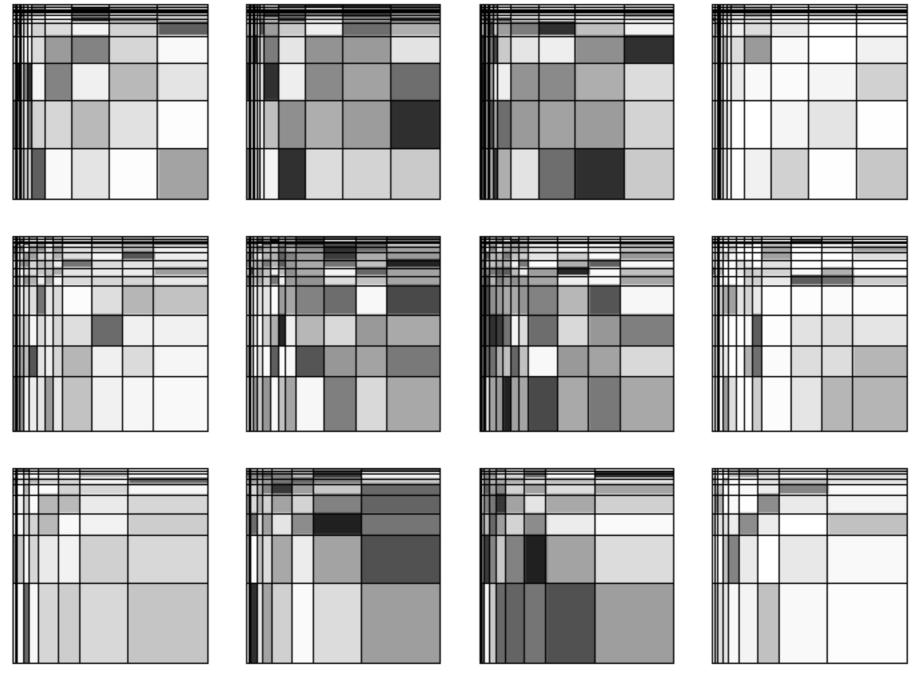
Dirichlet parameter a = [0, 0, 1, 0]







reordered

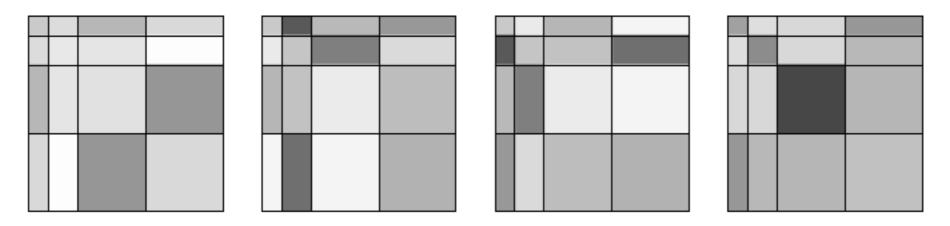


Dirichlet parameter a = [0.9, 2.0, 1.0, 0.5]

Inference via collapsed Gibbs sampling of cluster assignments

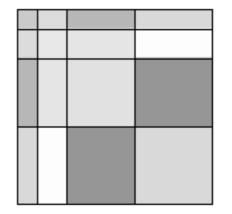
$$p(z_i|z_{-i},G) \propto p(z_i|z_{-i})p(G|z_i,z_{-i})$$
 cluster assignment of vertex i cluster assignments of all vertices except i

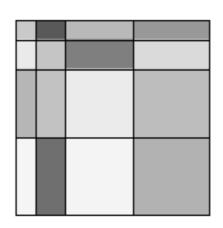
Experiments using synthetic data

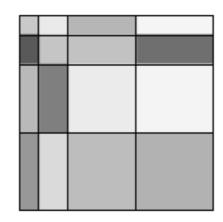


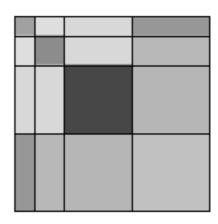
Dirichlet parameter a = [1, 1, 1, 1]

Random digraphon



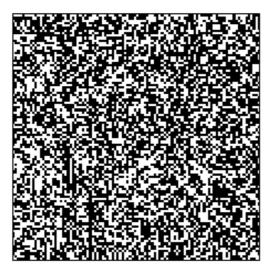




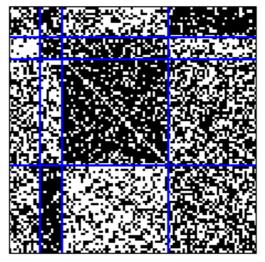


Dirichlet parameter a = [1, 1, 1, 1]

Random sample, 100 vertices

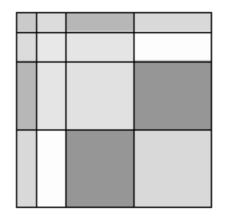


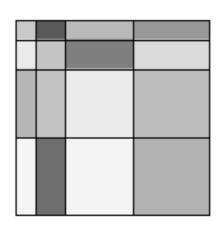
original ordering

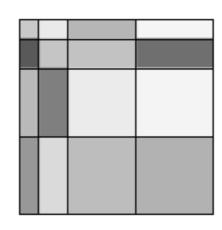


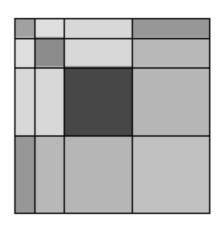
resorted by increasing uniform random variables

Random digraphon



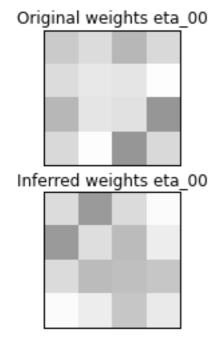


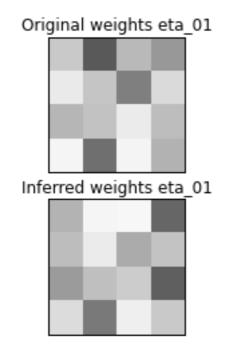


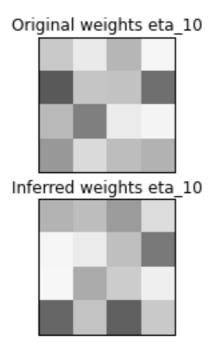


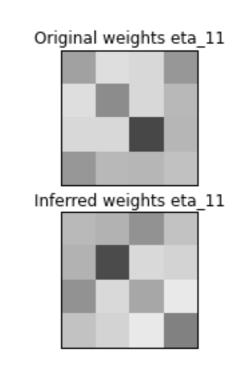
Dirichlet parameter a = [1, 1, 1, 1]

Collapsed Gibbs sampling

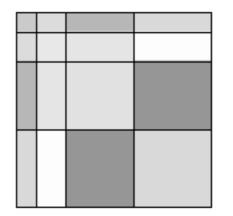


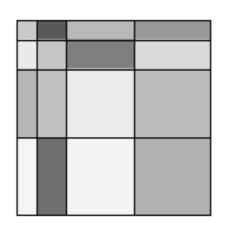


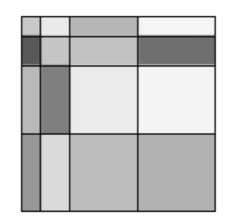


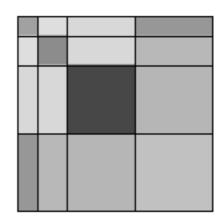


Random digraphon



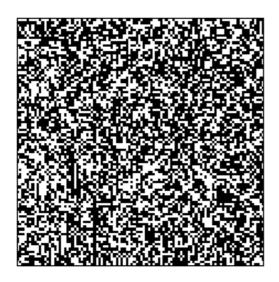




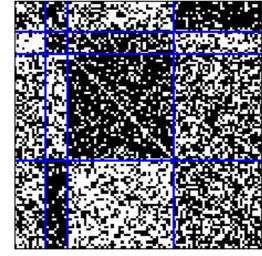


Dirichlet parameter a = [1, 1, 1, 1]

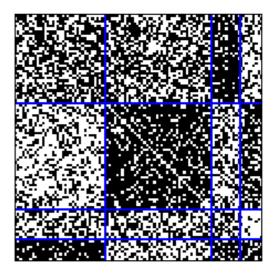
Collapsed Gibbs sampling



original ordering

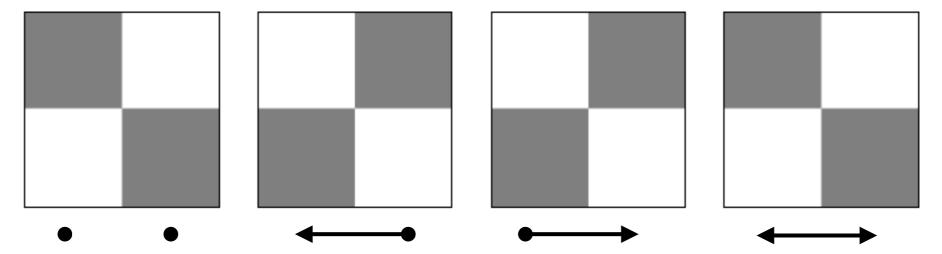


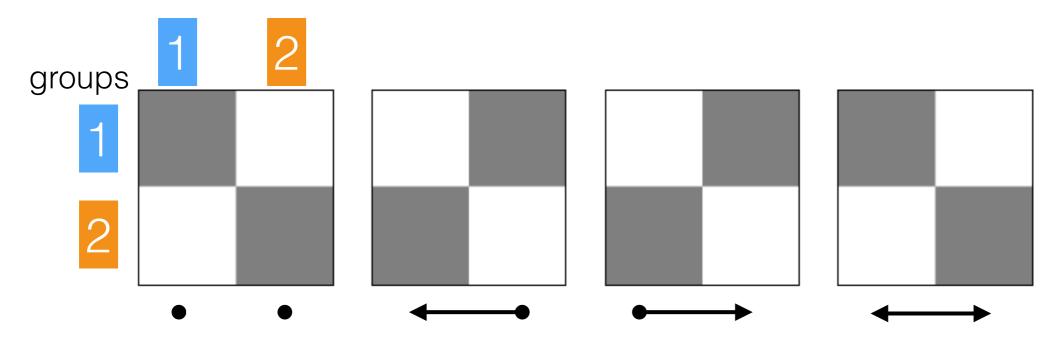
resorted by increasing uniform random variables



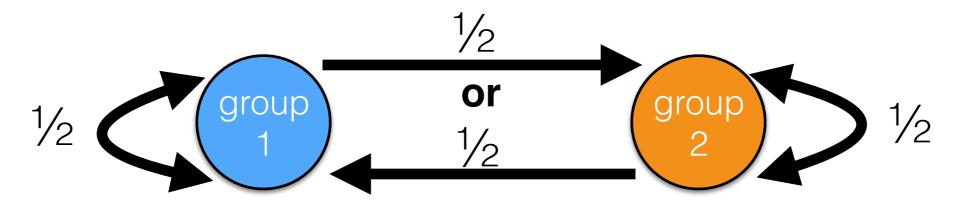
resorted by inferred cluster

Random digraphon: ER + tournament

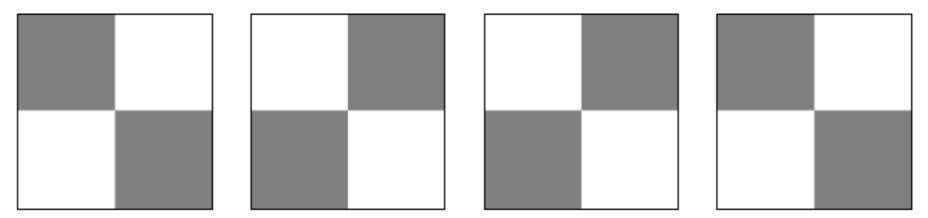




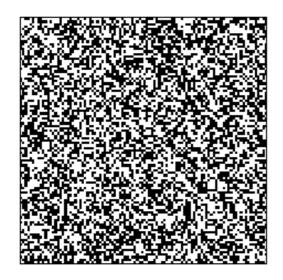
Schematic of the sampled digraph:



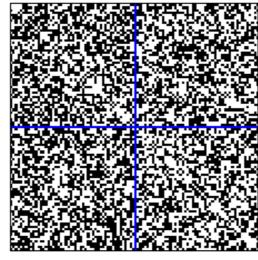
Random digraphon: ER + tournament



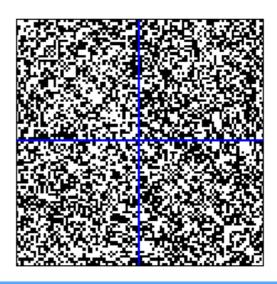
Collapsed Gibbs sampling for this model



original ordering

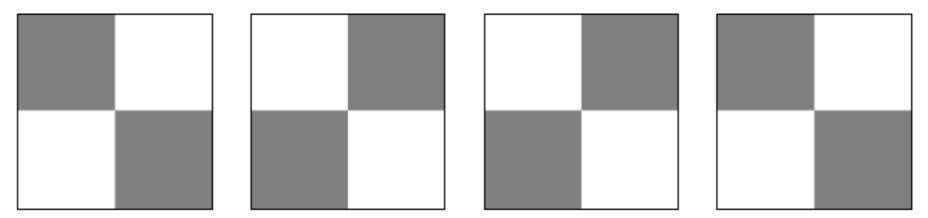


resorted by increasing uniform random variables

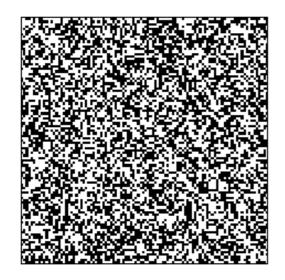


resorted by inferred cluster

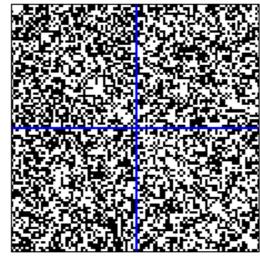
Random digraphon: ER + tournament



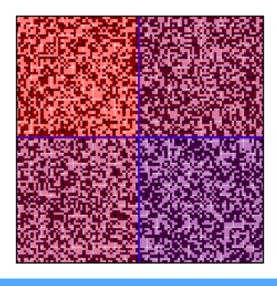
Collapsed Gibbs sampling for this model



original ordering

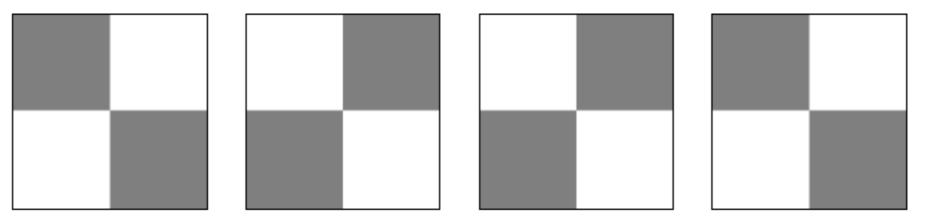


resorted by increasing uniform random variables

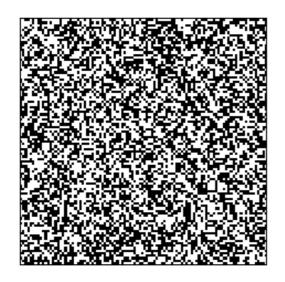


resorted by inferred cluster

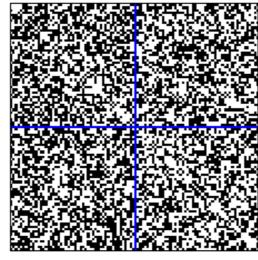
Random digraphon: ER + tournament



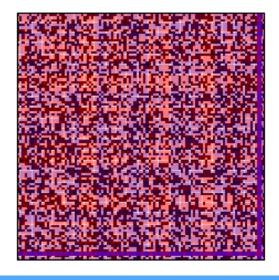
Collapsed Gibbs sampling for the infinite relational model



original ordering



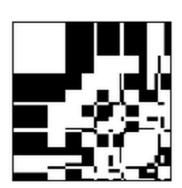
resorted by increasing uniform random variables



resorted by inferred cluster

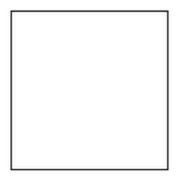
Conclusions

- Summary
- Discussion:









- other types of block models:
 - could consider other partitions, e.g., Pitman-Yor
- other priors, e.g., Gaussian process (as in Lloyd et al.)
- Aldous–Hoover already describes exchangeable hypergraphs
- sparsity

References

- D. J. Aldous. Representations for partially exchangeable arrays of random variables. *J. Multivariate Anal.*, 11(4): 581–598, 1981.
- P. Diaconis and S. Janson. Graph limits and exchangeable random graphs. *Rend. Mat. Appl.* (7), 28(1):33–61, 2008.
- E. Glasner and B. Weiss, Minimal actions of the group S(Z) of permutations of the integers, *Geom. Funct. Anal.* 12(5):964–988, 2002.
- D. N. Hoover. Relations on probability spaces and arrays of random variables. Preprint, Institute for Advanced Study, Princeton, NJ, 1979.
- C. Kemp, J. B. Tenenbaum, T. L. Griffiths, T. Yamada, and N. Ueda. Learning systems of concepts with an infinite relational model. In *Proc. 21st Nat. Conf. Artificial Intelligence (AAAI–06)*, 2006.
- J. R. Lloyd, P. Orbanz, Z. Ghahramani, and D. M. Roy. Random function priors for exchangeable arrays with applications to graphs and relational data. In *Adv. Neural Inform. Process. Syst. (NIPS)* 25:1007–1015, 2012.
- L. Lovász. Large networks and graph limits, vol. 60 of American Math. Soc. Colloq. Publ. American Math. Soc., Providence, RI, 2012.
- P. Orbanz and D. M. Roy. Bayesian models of graphs, arrays and other exchangeable random structures. *IEEE Trans. Pattern Anal. Mach. Intell.*, 37(2):437–461, 2015.
- Y. J. Wang, and G. Y. Wong. Stochastic blockmodels for directed graphs. *J. American Statist. Assoc.*, 82(397), 8–19, 1987.