W-graphs and their inference

(with emphasize en variational Bayes)

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Outline

Exchangeable graphs

W-graph & graphon function

Statistical inference

Variational Bayes inference of W-graph

From graphon to residual graphon

Some notations

Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$: $\mathcal{V}$ = vertices $:= \{1, \dots n\}$, $\mathcal{E}$ = edges $\subset \mathcal{V} \times \mathcal{V}$

Adjacency matrix $Y = [Y_{ij}]$:

$$Y : n \times n, \qquad Y_{ij} = \mathbb{I}\{(i,j) \in \mathcal{E}\}$$

Random graph: defined by the joint distribution of all edges

$$p(Y) = p\left([Y_{ij}]\right)$$

Undirected graph: $Y_{ij} = Y_{ji}$

Exchangeability

Classical exchangeability: for any permutation σ

$$P([Y_i = y_i]) = P([Y_i = y_{\sigma(i)}]).$$

Joint exchangeability for two dimensional arrays [9]:

$$P([Y_{ij}] = [y_{ij}]) = P([Y_{ij}] = [y_{\sigma(i)\sigma(j)}])$$

for any permutation σ (applied to both i and j).

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(Separate exchangeability: $P([Y_{ij}] = [y_{ij}]) = P([Y_{ij}] = [y_{\sigma(i)\tau(j)}])$
for any permutations σ and τ $\longrightarrow$ directed graphs.)

Aldous-Hoover theorem

Theorem: $Y = [Y_{ij}]$ is exchangeable iff there exists $F : [0,1]^3 \mapsto \{0,1\}$,

$$[Y_{ij}] \stackrel{d}{=} [F(U_i, U_j, U_{ij})]$$

where $(U_i)_i$ and $(U_{ij})_{i,j}$ are iid $\mathcal{U}[0,1]$.

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Properties:

- The Y_{ij}'s are not independent (because of the U_i's and U_j's)
- The Y_{ij}'s are conditionally independent given the U_i's:

$$[Y_{ij}]|(U_i = u_i)_i \stackrel{d}{=} [F(u_i, u_j, U_{ij})]$$

Some exchangeable random graphs

State-space models:

$$\begin{aligned} \{Z_i\}_i \text{ iid} &\sim \pi \\ \{Y_{ij}\}_{ij} \text{ indep.} \mid \{Z_i\}_i &\sim \mathcal{B}[\gamma(Z_i, Z_j)] \end{aligned}$$

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- Latent space [13]*: $Z_i \in \mathbb{R}^d, \quad \gamma(Z_i, Z_j) = f(\|Z_i - Z_j\|)$
- Model-based clustering [12]: $\pi =$ Gaussian mixture,
- Stochastic bloc-model (SBM) [14,23]: $\pi = \mathcal{M}, \quad \gamma = [\gamma_{k\ell}]$
- Continuous version of SBM [8]*: $Z_i \in \mathcal{S}^d$
- W-graph [20,9]: $\pi = \mathcal{U}_{[0,1]}$

See [21] for a statistical review + [3] for theoretical properties.

(*): Z_i not explicitly random

W-graph

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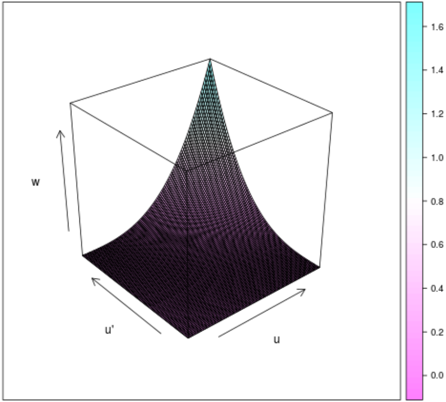
W-graph

Graphon function $w(u, u')$



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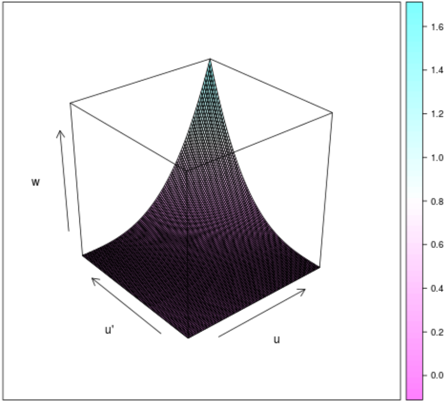
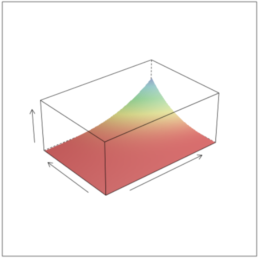


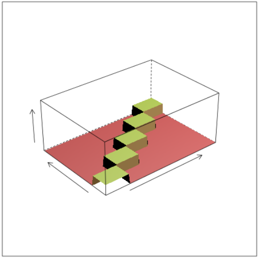
Aldous-Hoover representation: $F(U_i, U_j, U_{ij}) = \mathbb{I}\{U_{ij} < w(U_i, U_j)\}$

Some ideal graphons

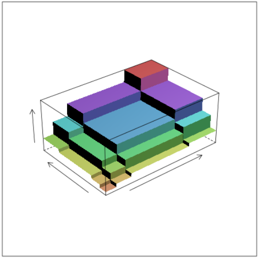
'Scale free'



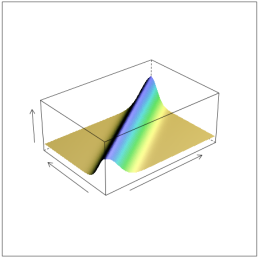
Community



SBM



Small world



W-graph as limit for dense graphs

Asymptotic framework: (a crude rephrasing of [20,9])

- $(\mathcal{G}_n)$ = sequence of exchangeable graphs with increasing size (say n)
- $t(F, G)$ = number of occurrences of subgraph F (with k nodes) in G normalized by $n_{[k]}$.

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Convergence: If for any finite set of fixed subgraphs $(F_1, \dots F_m)$, $(t(F_1, \mathcal{G}_n), \dots t(F_m, \mathcal{G}_n))$ converge in distribution,
then

- there exist a W-graph $\mathcal{G}$ such that $(\mathcal{G}_n) \xrightarrow{d} \mathcal{G}$;
- for any fixed F, $\mathbb{E}t(F, \mathcal{G}_n) \longrightarrow f(F)$ where

$$f(F) = \int_{[0,1]^k} \prod_{(i,j) \in \mathcal{E}(F)} w(u_i, u_j) \, \mathrm{d}u_1 \dots \, \mathrm{d}u_k$$

Some comments

Questions

- How strong is the condition

$$(t(F_1, \mathcal{G}_n), \dots t(F_m, \mathcal{G}_n)) \text{ converge in distribution?}$$

- Does it hold for most popular state-space models?
- Does it hold for other popular state graph models (e.g. ERGM [10])?

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- Does it hold for other popular state graph models (e.g. ERGM [10])?

Comments: If so

- One should be able to derive the graphon of any of these models.
- Only pairwise interactions (asymptotically) matter.
- More complex patterns (e.g. triangles in ERGM) are (asymptotically) useless.

Identifiability

Obvious identifiability problem: consider $\phi : [0, 1] \mapsto [0, 1]$ measure preserving, then the two graphons

$$w(u, v) \qquad \text{and} \qquad w'(u, v) = w(\phi(u), \phi(v))$$

give raise to the same random graph [9,26].

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Degree function: Denoting $D_i = \sum_{j \neq i} Y_{ij}$, $\mathbb{E}(D_i | U_i = u) = (n-1) g(u)$,

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Identifiability condition [2,26,6]:

$$g(u) \text{ strictly increasing.}$$

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Infering w

Main issues

- W-graph is a state-space for graph = incomplete data model
  $\rightarrow$ Specificity of graph models: $p([U_i]|Y)$ intractable[1].

- W-graph is a graph model
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Specificity of W-graph

- Recent interest in the statistical community (since 2014)
  $\rightarrow$ but explosion since then.
- Main interest = flexibility of w
  $\rightarrow$ Mostly non or semi-parametric methods.

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Low-rank connexion probability matrix

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Some references:

- [7]: thresholding the singular values of Y + bounds on the MSE
- [26]: same principle + smoothing of the resulting graphon.

SBM-based approximations

SBM = W-graph with block-wise constant graphon function.

General strategy:

1. Assign nodes to block (+ order the blocks wrt degree)
2. Estimate $w(u, v)$ with the empirical between block connectivity

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A series of works:

- [24]: Constant block width h (after degree ordering) + bound on $MISE(\widehat{w})$[2]
- [6]: Same idea + smoothing between neighbor blocks
- [16,11]: Convergence rate for the least-square estimate[3] of a sparse graphon $w_n(u, v) = \rho_n w(u, v)$
- [18]: Bayesian model averaging of SBM with increasing number of blocks.
- And more [5,4]...

---

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Variational Bayes inference: General principle

$Y =$ observed data, $Z =$ latent variable, $\theta =$ parameter.

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Typically [15,1,22,25]

$$\widetilde{p} = \arg\min_{q \in \mathcal{Q}} D[q(\cdot) \parallel p(\cdot|Y)]$$

- $D[q \parallel p] = KL[q \parallel p]$
- $q(\theta) = \mathcal{N}$
- $q(Z) = \prod_i q_i(Z_i)$
- $q(\theta, Z) = q(\theta)q(Z)$.

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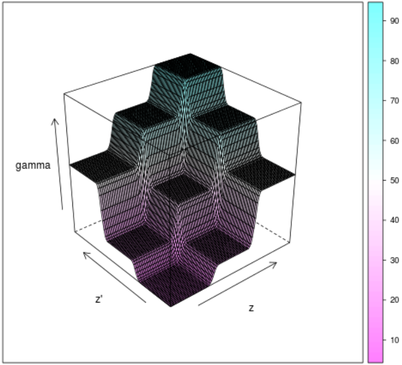
Inferred graphon with SBM_K



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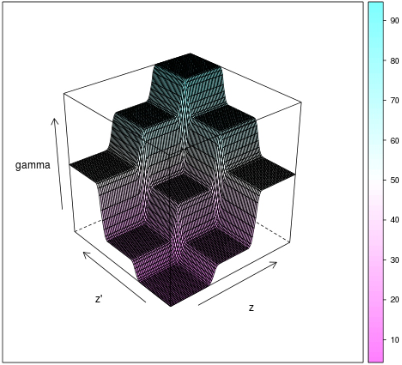

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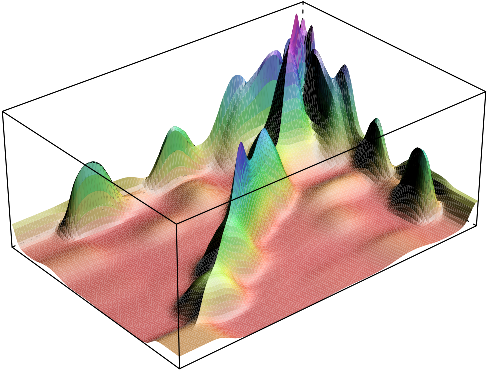
Bayesian model averaging [18]:

$$\widetilde{\mathbb{E}}[w(u,v)] = \sum_K \widetilde{P}(K)\widetilde{\mathbb{E}}_K^{SBM}[w(u,v)]$$

How to interpret a graphon?

French political blogs: $n = 196$ nodes [18]



$\rightarrow$ Depicts the heterogeneity of the network.

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Goodness of fit (GOF): Check if $\omega(u, v) = \text{cst} \qquad (= \beta_0)$

Goodness-of-fit as model comparison

Auxiliary model M_K:

$$\text{logit } P(Y_{ij} = 1 | U_i, U_j, K) = \omega_K^{SBM}(U_i, U_j) + x_{ij}^\intercal \beta.$$

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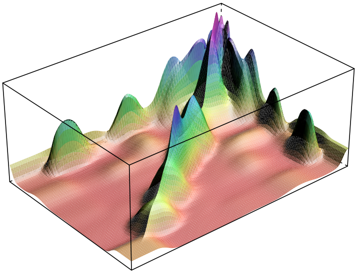
Actually: use $\widetilde{P}(H_0)$ and $\widetilde{P}(M_1)$.

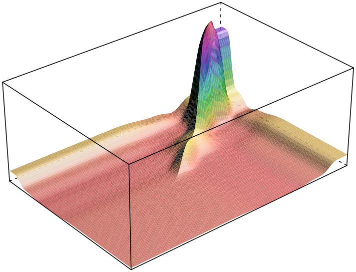
Political blog network

$n = 196$ blogs ($N = 19110$ pairs), 3 covariates, density $= .075$

Inferred graphon (no covariate)



Residual graphon (3 covariates)

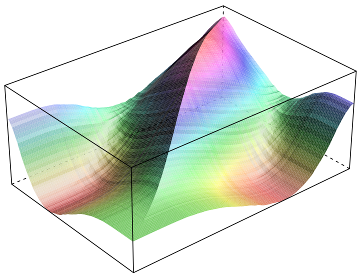


$\widetilde{P}(H_0) \simeq 10^{-172}$

Florentine business

$n = 16$ families ($N = 120$ pairs), 3 covariates, density $= .12$

Inferred graphon (no covariate)



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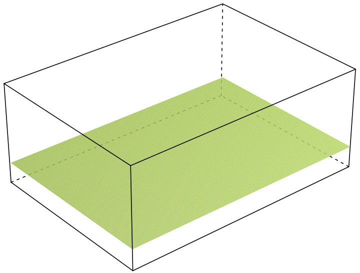

$\widetilde{P}(H_0) = .991$

Some more examples

network	size (n)	nb. covariates (d)	density	$\hat{p}(H_0 \mid Y)$
Blog	196	3	0.075	3e-172
Tree	51	3	0.54	2e-115
Karate	34	8	0.14	3e-2
Florentine (marriage)	16	3	0.17	0.995
Florentine (business)	16	3	0.125	0.991
Faux Dixon High	248	17	0.02	1
CKM	219	39	0.015	1
AddHealth 67	530	21	0.007	2e-25

Conclusion

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Variational Bayes inference and GOF

- R package on `github.com/platouche/gofNetwork` (soon on CRAN)
- Strongly relies on variational Bayes approximation of the posteriors.
  $\longrightarrow$ VBEM asymptotically accurate for logistic regression and SBM
  $\longrightarrow$ No clue about accuracy in the combined model.

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