On Graphon Estimation

Nicolas Verzelen

INRA, Montpellier

(Based on Joint Work with Olga Klopp and Alexander Tsybakov)

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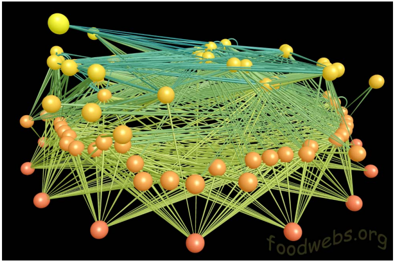
Network model

Network analysis is ubiquitous in social sciences, genomics, ecology,. . .



East-river trophic network [Yoon et al.(04)]

Objectives :

- Graph Visualization
- Backbone estimation
- Node clustering

Approach

- The modeling of real networks as random graphs.
- Model-based statistical analysis.

1 Graphon Model

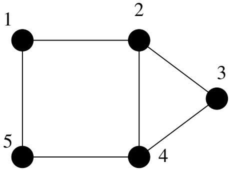
2 Towards Graphon Estimation

3 $\delta_\square$ and δ_2 Estimation of sparse Graphons

Graph Notation

A (simple, undirected graph) $\mathcal{G} = (\mathcal{E}, \mathcal{V})$ consists of

- a set of vertices $V = \{1, \ldots n\}$
- a set of edges $E \subset \{\{i, j\} : i, j \in V \text{ and } i \neq j\}$



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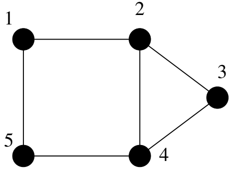


$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{pmatrix}$$

The corresponding adjacency matrix is denoted $\mathbf{A} = (\mathbf{A}_{i,j}) \in \{0,1\}^{n \times n}$, where $\mathbf{A}_{i,j} = 1 \Leftrightarrow (i,j) \in E$

Stochastic Block-Model (SBM) Holland et al. '80

A mixture model for random graphs : **K** classes.

SBM popular for clustering applications : generate graphs with a community structure

Latent labels : each node i belongs to class k with probability π_k :

$$\{\xi_i\}_i \text{ IID}, \ \xi_i \sim \mathcal{M}(1;\pi) \ ,$$

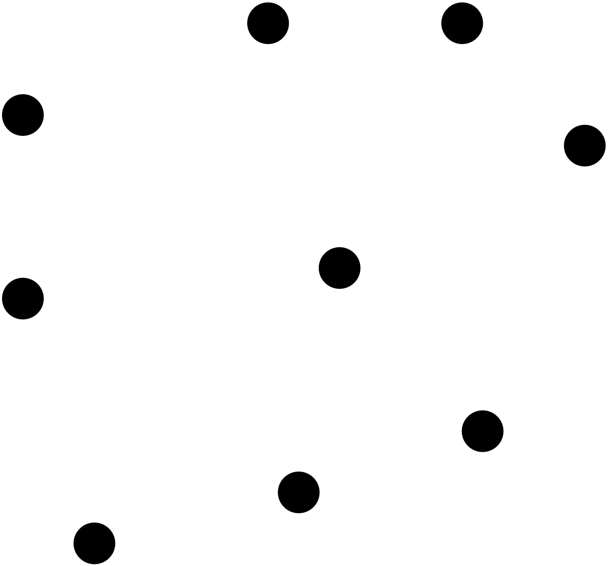
where $\pi = (\pi_1, \dots, \pi_K)$.

Observed edges : $(\mathbf{A}_{ij})$ are conditionally independent given the ξ_i's :

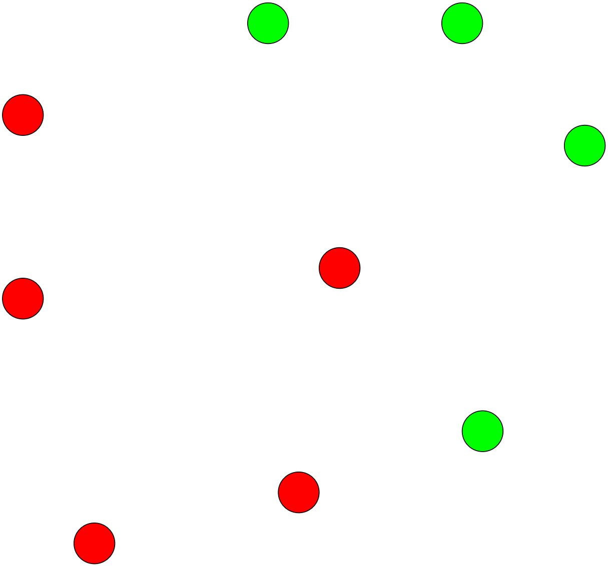
$$(\mathbf{A}_{ij} | \xi_i = k, \ \xi_j = l) \sim \mathcal{B}(\mathbf{Q}_{k,l})$$

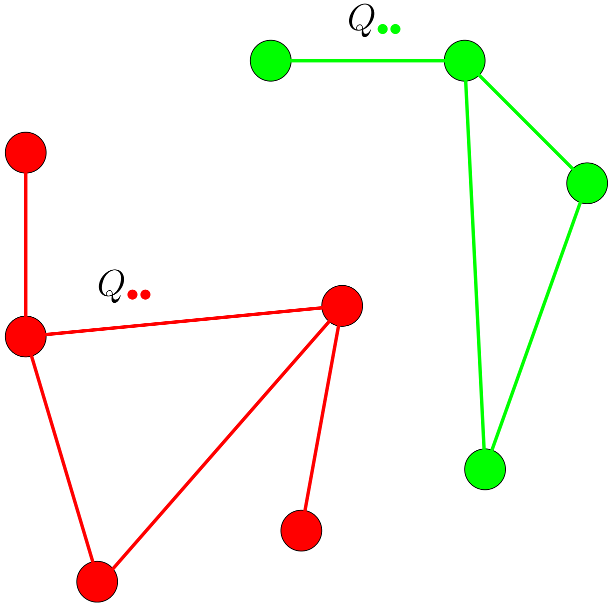
The symmetric $K \times K$ matrix $\mathbf{Q}$ is called the connectivity matrix.

(Basic approximation unit for more complex models)



Example

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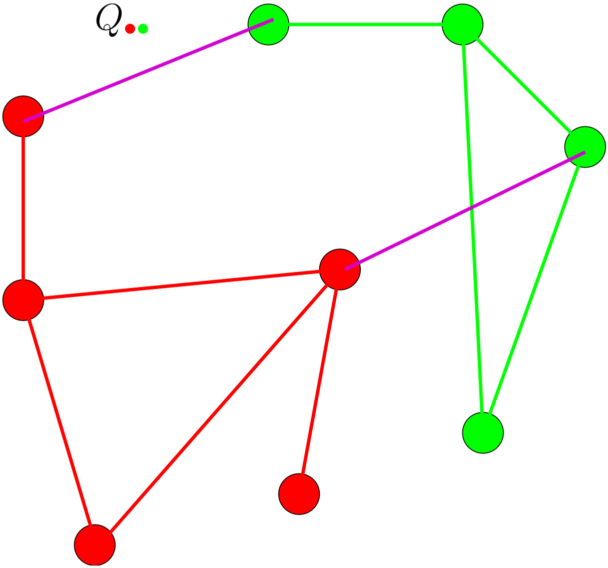

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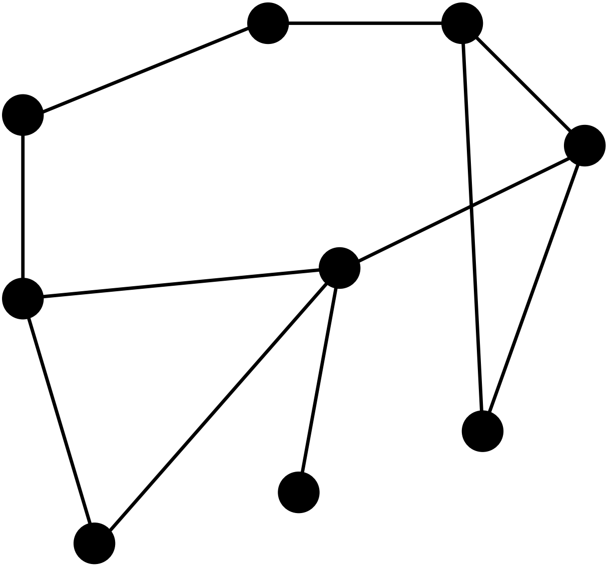
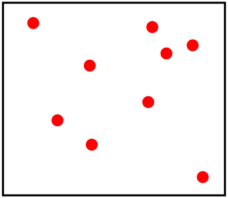


Definition

- ξ_i = unobserved position of node i in a latent space. e.g. $\xi_i \sim \mathcal{U}([0,1]^2)$
- Edges $\mathbf{A}_{ij}$ independent given ξ_i,

$$\mathbb{P}[\mathbf{A}_{ij} = 1] = \gamma(\|\xi_i - \xi_j\|_2$$

with $\gamma : \mathbb{R}^+ \to [0,1]$.



Latent space models (Hoff et al.,'02)

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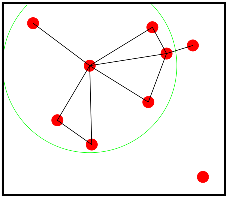

W-random Graph Model Diaconis & Janson('06)

SBM do not allow to analyze the fine structure of extremely large networks
$\rightsquigarrow$ **Non-parametric models**

Graphons

A graphon is a triplet (Ω, π, W) where :

- (Ω, π) is a Borel Probability space
- $W : \Omega \times \Omega \mapsto [0, 1]$ measurable

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W-Random graph

W-random graph model of size n associated to (Ω, π, W) :

- $\xi = (\xi_1, \ldots, \xi_n)$ are sampled on Ω according to π.
- For each $i < j$, $\mathbf{A}_{ij} = 1$ with probability $W(\xi_i, \xi_j)$.

Notation : $\mathbb{P}^n_W$ xorresponding distribution ($\mathbb{P}_W := \mathbb{P}^\infty_W$)
$\boldsymbol{\Theta}_0$ defined by $\boldsymbol{\Theta}_{ij} = W(\xi_i, \xi_j)$ for $i \neq j$

Remarks

- $\mathbb{E}[\mathbf{A}|\xi] = \boldsymbol{\Theta}_0 \rightsquigarrow$ cond. to ξ, inhomogeneous random graph with Matrix $\boldsymbol{\Theta}_0$.
- If W is a k step-function, $\mathbf{A}$ SBM with k blocks

Universality of W-random graph model.

Let $\underline{\mathbf{A}} : \mathbb{N} \times \mathbb{N} \to \{0,1\}$ symmetric = the adjacency function of an infinite graph
For τ permutation, $\underline{\mathbf{A}}^\tau$ defined by $\underline{\mathbf{A}}^\tau[i,j] = \underline{\mathbf{A}}[\tau(i), \tau(j)]$.

Joint Exchangeability

The distribution of $\underline{\mathbf{A}}$ is jointly exchangeable if

$$\underline{\mathbf{A}} \sim \underline{\mathbf{A}}^\tau \ , \qquad \text{for any permutation } \tau.$$

Theorem (Aldous-Hoover Representation Theorem('79))

If the distribution of $\underline{\mathbf{A}}$ is jointly exchangeable, then there exists μ such that

$$(\Omega, \pi, W) \sim \mu$$

$$[\underline{\mathbf{A}} | (\Omega, \pi, W)] \sim \mathbb{P}_W$$

$\rightsquigarrow$ W-random graph distribution correspond to extremal points of the set of jointly exchangeable distributions.

Sparse Graphons

For W-random graph, $\mathbb{E}_W[\#E] \asymp n^2 \rightsquigarrow$ Realized graphs are dense

Sparse Graphon Models

(Ω, π, W, ρ_n) with $\rho_n \to_{n\to\infty} 0$.

1. Sample ξ according to π
2. For each $i < j$, draw an edge between i and j with probability $\rho_n W(\xi_i, \xi_j)$

Other methods :

- L_p graphon (e.g Borgs et al.('15))
- Graphex (e.g.Veitch & Roy('16))

Objective

Given an observation $\mathbf{A}$, goal = infering the graphon (Ω, π, W) in some sense...

Caveats :

- Identifiability
- Loss functions
- Approximation class

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Lemma

(Ω, π, W) *graphon*
$\tau : (\Omega', \pi') \mapsto (\Omega, \pi)$ *measure-preserving*
W^τ *be such that* $W^\tau(x, y) := W(\tau(x), \tau(y))$*. Then* $\mathbb{P}_W = \mathbb{P}_{W^\tau}$*.*

Two Consequences :

- Triplet (Ω, π, W) is not identifiable
- Sufficient to consider graphons on $([0, 1], \lambda)$ [but problematic]
  $\rightsquigarrow \mathcal{W}$: space of graphons on $([0, 1], \lambda)$.

Identifiability (fd)

Even Restricting to $([0,1],\lambda)$, the topology of a network **invariant** wrt node labeling change :

Weak isomorphism

Two graphons U and W are **weakly isomorphic** if there exist measure preserving maps ϕ, $\psi : [0,1] \to [0,1]$ such that $U^{\phi} = W^{\psi}$ almost everywhere.

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Proposition (Lovász('12))

$\mathbb{P}_U = \mathbb{P}_W$ *if and only if* U *and* W *are weakly isomorphic.*

$\rightsquigarrow$ one can only perform inference in $\widetilde{\mathcal{W}}$ (equivalence classes of $\mathcal{W}$ wrt weak isomorphism)

Distance betw. **graphs** $\rightsquigarrow$ Distance betw.**graphons** $\rightsquigarrow$ Distance bet. **equivalence classes**

Distance on Graphs :

$\|\mathbf{A}-\mathbf{B}\|_2 := \frac{1}{n}\sqrt{\sum_{ij}(\mathbf{A}_{ij}-\mathbf{B}_{ij})^2}$ $\rightsquigarrow$ Frobenius distance

$\|\mathbf{A}-\mathbf{B}\|_\square := \frac{1}{n^2}\max_{S,T\subset[n]}\left|\sum_{i\in S,j\in T}\mathbf{A}_{ij}-\mathbf{B}_{ij}\right|$ $\rightsquigarrow$ Cut Distance

Metrics/Loss functions on $\widetilde{\mathcal{W}}$

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Norms on Graphons :

$\|W\|_2 := [\int_{[0,1]^2} W^2(x,y)dxdy]^{1/2}$ $\rightsquigarrow$ Frobenius norm

$\|W\|_\square := \sup_{S,T\subset[0,1]}\left|\int_{S\times T} W(x,y)dxdy\right|$ $\rightsquigarrow$ Cut norm (cornerstone of graph limits)

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Distances on $\widetilde{\mathcal{W}}$.

$\mathcal{M}$: Measure-preserving bijections $\tau : [0,1]\to[0,1]$

l_2 distance $\delta_2(W,W_1) := \inf_{\tau\in\mathcal{M}}\|W-W_1^\tau\|_2$

Cut distance $\delta_\square(W,W_1) := \inf_{\tau\in\mathcal{M}}\|W-W_1^\tau\|_\square$

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These metrics are not equivalent : $\delta_\square(W,\widehat{W}) \leq \delta_2(W,\widehat{W})$

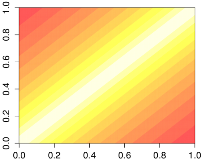
Regularity Lemma and approximation by SBMs

Proposition (Szemerédi ('75), Frieze and Kannan ('99))

For any $W \in \mathcal{W}$ and any k, there exists a k-step graphon W_k such that

$$\|W - W_k\|_{\square} \lesssim \frac{1}{\sqrt{\log(k)}}$$

This rate is universal!



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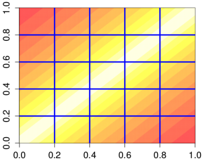

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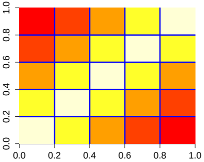
Obviously false for δ_2 : similar to histograms in classical Nonparametric Estimation



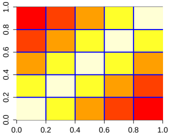
Estimating $f_0 = \rho_n W_0$

$$\rho_n W_0 \longrightarrow \mathbf{\Theta}_0 \longrightarrow \mathbf{A}$$

General Scheme :

1. Estimating the matrix $\mathbf{\Theta}_0 := \mathbb{E}[\mathbf{A}|\xi]$ by $\widehat{\mathbf{\Theta}}$.
2. From matrix to graphon. Given $\mathbf{\Theta}$, define the **empirical graphon** $\widetilde{f}_{\mathbf{\Theta}}$ as the n piecewise constant function :

$$\widetilde{f}_{\mathbf{\Theta}}(x,y) = \mathbf{\Theta}_{\lceil nx \rceil, \lceil ny \rceil}, \qquad x, y \in [0,1]$$



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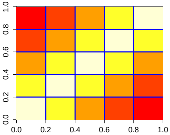

Lemma

For any estimator $\widehat{\mathbf{\Theta}}$ and any norm N,

$$\mathbf{E}\left[\delta_N(\widetilde{f}_{\widehat{\mathbf{\Theta}}}, f_0)\right] \leq \mathbf{E}\left[\|\widehat{\mathbf{\Theta}} - \mathbf{\Theta}_0\|_N\right] + \underbrace{\mathbf{E}\left[\delta_N\left(\widetilde{f}_{\mathbf{\Theta}_0}, f_0\right)\right]}_{\text{agnostic error}}$$

Estimating Θ_0

- Raw data : $\mathbf{A}$
- Restricted Least Squares estimator : (RLS) Wolfe & Olhlede ('13), Borgs et al.('15), Klopp, Tsybakov, V.('17), Gao et al.('17)

$$\widetilde{\mathbf{\Theta}}_\lambda \in \arg \min_{\mathbf{\Theta} \in \mathrm{SBM}(k):\ \|\mathbf{\Theta}\|_\infty \leq \mathbf{r}} \|\mathbf{A} - \mathbf{\Theta}\|_2^2,$$

where $r \in (0,1)$ and $\mathrm{SBM}(k)$ space of k block-constant matrix.
($\widehat{\mathbf{\Theta}}_k^r$ is not polynomial-time computable)

- Singular Value Thresholding : $\widetilde{\mathbf{\Theta}}_\lambda$ e.g. Chatterjee('12), Klopp & V.('17)

$$\widetilde{\mathbf{\Theta}}_\lambda := \sum_{j:\sigma_j(\mathbf{A}) \geq \lambda} \sigma_j(\mathbf{A}) u_j(\mathbf{A}) v_j(\mathbf{A})^T \ ,$$

Probability Matrix Estimation in $\|.\|_2$

Theorem (Oracle inequality Klopp, Tsybakov, V.('17))

For any $\mathbf{\Theta}_0$ *such that* $\|\mathbf{\Theta}_0\|_\infty \leq r$*,*

$$\mathbb{E}\left[\|\widehat{\mathbf{\Theta}}^r_k - \mathbf{\Theta}_0\|_2^2\right] \lesssim \min_{\mathbf{\Theta}\in\mathrm{SBM}(k)} \|\mathbf{\Theta}_0 - \mathbf{\Theta}\|_2^2 + r\left(\frac{\log k}{n} + \frac{k^2}{n^2}\right)$$

(Minimax optimal over $\mathrm{SBM}(k) \cap \mathcal{B}_\infty(r)$) (Gao et al. ('15))

Two terms :

- $\frac{k^2}{n^2} \rightsquigarrow$ parametric rate $(k(k+1)/2$ parameter to estimate)
- $\frac{n\log(k)}{n^2} \rightsquigarrow$ clustering rate (of order k^n possible partitions)

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SVT estimator

Fix $\lambda = c\sqrt{n\|\mathbf{\Theta}_0\|_\infty}$. For all k,

$$\mathbb{E}[\|\widetilde{\mathbf{\Theta}}_\lambda - \mathbf{\Theta}_0\|_2^2] \lesssim \min_{\mathbf{\Theta} \in \mathrm{SBM}(k)} \|\mathbf{\Theta}_0 - \mathbf{\Theta}\|_2^2 + \frac{\|\mathbf{\Theta}_0\|_\infty k}{n},$$

Loss of order $\frac{k}{\log(k)} \wedge \frac{n}{k}$ wrt RLS estimators

Best known polynomial time bound

δ_2 Graphon Estimation for k-step functions

$\mathcal{W}[k]$: Collection of k-**Step function graphons**
Here $f_0 = \rho_n W_0$ with $W \in \mathcal{W}[k]$

Proposition

$$\mathbb{E}\left[\delta^2\left(\widetilde{f}_{\boldsymbol{\Theta}_0}, f_0\right)\right] \lesssim \rho_n^2 \sqrt{\frac{k}{n}}$$

If $\rho_n \leq r$ then for RLS

$$\mathbb{E}\left[\delta^2\left(f_{\widehat{\boldsymbol{\Theta}}_k^r}, f_0\right)\right] \lesssim \rho_n \left(\frac{k^2}{n^2} + \frac{\log(k)}{n}\right) + \rho_n^2 \sqrt{\frac{k}{n}}$$

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For SVT

$$\mathbb{E}\left[\delta^2\left(f_{\widetilde{\mathbf{\Theta}}_\lambda}, f_0\right)\right] \lesssim \rho_n \frac{k}{n} + \rho_n^2 \sqrt{\frac{k}{n}}$$

(RLS is Minimax optimal (up to possible $\log(k)$ term)) Klopp et al. ('17)

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For SVT

$$\mathbb{E}\left[\delta^2\left(f_{\widetilde{\mathbf{\Theta}}_\lambda}, f_0\right)\right] \lesssim \rho_n\frac{k}{n} + \rho_n^2\sqrt{\frac{k}{n}}$$

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(i) **Weakly sparse graphs :** $\Longrightarrow$ the agnostic error dominates.

(ii) **Moderately sparse graphs :** $\Longrightarrow$ the Probability matrix estimation error dominates

(iii) **Highly sparse graphs :** The null estimator $\tilde{f} \equiv 0$ is of smaller order

Probability Matrix Estimation in cut norm

Proposition

For any probability matrix $\mathbf{\Theta}_0$ such that $\|\mathbf{\Theta}_0\|_\infty \geq 1/n$,

$$\mathbf{E}\left[\|\mathbf{A} - \mathbf{\Theta}_0\|_\square\right] \leq 12\sqrt{\frac{\|\mathbf{\Theta}_0\|_\infty}{n}}$$

- Valid for all matrices $\mathbf{\Theta}_0$. Optimal convergence rate (even for simple classes such as two-block matrices)
- More refined estimators (SVT) do not decrease the performances but RLS may be biased.

Graphon Estimation in Cut distance

Theorem ((Consequence of Szemeredi's Lemma) Lovász, '12)

For all W_0 with $\rho_n = 1$, one has whp

$$\delta_{\square}\left(\tilde{f}_{\mathbf{A}}, W_0\right) \lesssim \frac{1}{\sqrt{\log(n)}} .$$

Valid for all graphons !

Theorem (Klopp and V., '17)

For all $W_0 \in \mathcal{W}[k]$ and $\rho_n > 0$, we have

$$\mathbf{E}_{W_0}\left[\delta_{\square}\left(\widetilde{f}_{\mathbf{A}}, f_0\right)\right] \lesssim \rho_n \min\left(\sqrt{\frac{k}{n\log(k)}}, \frac{1}{\sqrt{\log(n)}}\right) + \sqrt{\frac{\rho_n}{n}}$$

- Similar bound for the SVT estimator $\widetilde{f}_{\widetilde{\mathbf{\Theta}}_\lambda}$
- **This convergence rate is optimal**

Graphon Estimation in Cut distance

Theorem ((Consequence of Szemeredi's Lemma) Lovász, '12)

For all W_0 with $\rho_n = 1$, one has whp

$$\delta_{\square}\left(\tilde{f}_{\mathbf{A}}, W_0\right) \lesssim \frac{1}{\sqrt{\log(n)}}\ .$$

Valid for all graphons !

Theorem (Klopp and V., '17)

For all $W_0 \in \mathcal{W}[k]$ and $\rho_n > 0$, we have

$$\mathbf{E}_{W_0}\left[\delta_{\square}\left(\widetilde{f}_{\mathbf{A}}, f_0\right)\right] \lesssim \rho_n \min\left(\sqrt{\frac{k}{n\log(k)}}, \frac{1}{\sqrt{\log(n)}}\right) + \sqrt{\frac{\rho_n}{n}}$$

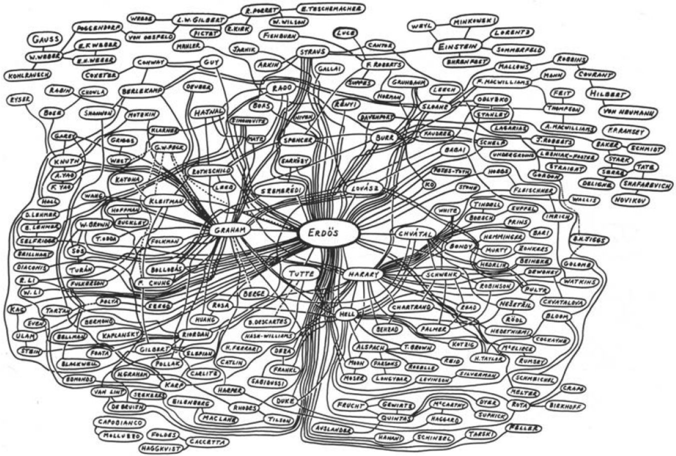
- Similar bound for the SVT estimator $\widetilde{f}_{\widetilde{\mathbf{\Theta}}_\lambda}$
- **This convergence rate is optimal**

(i) **Weakly sparse graphs** Agnostic error dominates.

(ii) **Moderately sparse graphs** Probability Matrix Estimation error dominates.

Discussion

- Non-parametric viewpoint on network analysis
- Identifiability Caveats
- Importance of the metric choice
- Good behavior of universal Singular Value Thresholding estimator.
- Computational barriers for estimation in δ_2 ?
- Less results for L_p graphons (Borgs et al.'16) and graphex
- Incorporating some geometry into estimation
  $\rightsquigarrow$ Functional Estimation (e.g. Issartel'17+)



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Thank You !