Sparse Network Estimation

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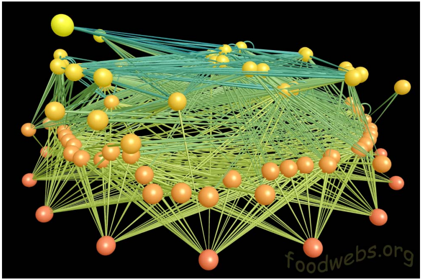
Network model

Network analysis has become an important research field driven by applications in social sciences, computer sciences, statistical physics, biology,. . .



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

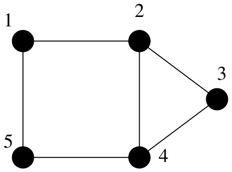
Approach

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

Graph Notations

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

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



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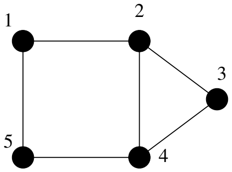

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{pmatrix}$$

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

Sparsity

Main integral characteristics

- number of vertices n
- number of edges $|E|$

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Maximal number of edges

$$\frac{n(n-1)}{2}$$

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Maximal number of edges

$$\frac{n(n-1)}{2}$$

- Dense graph $|E| \asymp n^2$
- Real world networks are sparse : $|E| = o(n^2)$
  - more difficult to handle

Stochastic Block-Model (SBM) Holland et al. (1980)

- Fit observed networks to parametric or non-parametric models of random graphs.
- **SBM** popular in applications: it allows to generate graphs with a community structure
  - Parameters:
    - Partition of n nodes into k disjoint groups $\{C_1, \dots, C_k\}$
    - Symmetric $k \times k$ matrix Q of inter-community edge probabilities.
  - Any two vertices $u \in C_i$ and $v \in C_j$ are connected with probability Q_{ij}.
  - **Regularity Lemma:** basic approximation units for more complex models.

Non-parametric Model

- SBM does not allow to analyze the fine structure of extremely large networks, in particular when the number of groups is growing.
- Non-parametric models of random graphs: **Graphon Model**
  - Graphons are symmetric measurable functions

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

  - Play a central role in the recent theory of graphs limits: every graph limit can be represented by a graphon.
  - Graphons give a natural way of generating random graphs.

Graphon Model

- **Graphon Model:**
  - $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_n)$ are latent i.i.d. uniformly distributed on $[0, 1]$.

$$\boldsymbol{\Theta}_{ij} = W_0(\xi_i, \xi_j).$$

  - The diagonal entries $\boldsymbol{\Theta}_{ii}$ are zero and $\boldsymbol{\Theta}_0 = (\boldsymbol{\Theta}_{ij})$
  - Given $\boldsymbol{\Theta}_0$ the graph is sampled according to the **inhomogeneous random graph model**:
    - ⋆ vertices i and j are connected by an edge with probability $\boldsymbol{\Theta}_{ij}$ independently from any other edge.
  - If W_0 is a step-function with k steps, the graph is distributed as a SBM with k groups.

Sparse Graphon Model

- The expected number of edges $\asymp n^2 \;\Rightarrow\;$ **dense** case.
- In real life networks often **sparse**
- **Sparse Graphon Model:**
  - Take $\rho_n > 0$ such that $\rho_n \to 0$ as $n \to \infty$.
  - The adjacency matrix $\mathbf{A}$ is sampled according to graphon W_0 with scaling parameter ρ_n:

$$\mathbf{\Theta}_{ij} = \rho_n W_0(\xi_i, \xi_j),\; i < j.$$

  - $\rho_n =$ "expected proportion of non-zero edges",
  - the number of edges is of the order $O(\rho_n n^2)$,
    - ★ $\rho_n = 1$ dense case
    - ★ $\rho_n = 1/n$ very sparse

Network Model

From a single observation of a graph

Problem 1:

Estimate the matrix of connection probabilities $\mathbf{\Theta}_0$

and

Problem 2:

Estimate the sparse graphon function $f_0(x, y) = \rho_n W_0(x, y)$

- We observe the $n \times n$ adjacency matrix $\mathbf{A} = (\mathbf{A}_{ij})$ of a graph
- $\mathbf{A}$ has been sampled according to the inhomogeneous random graph model with a fixed matrix $\mathbf{\Theta}_0$ or to the graphon model with graphon W_0
- Given a single observation $\mathbf{A}$, we want to estimate $\mathbf{\Theta}_0$ or f_0.

Graphon: invariance with respect to the change of labeling

- Graphon estimation is **more challenging** than probability matrix estimation
- Multiple graphons can lead to the same distribution on the space of graphs of size n.
- The topology of a network is **invariant with respect to any change of labeling** of its nodes
- We consider **equivalence classes** of graphons defining the same probability distribution on random graphs.

Loss function for graphon estimation

- Consider a sparse graphon $f(x,y) = \rho_n W(x,y)$
- $\tilde{f}(x,y)$ estimator of $f(x,y)$
- The squared error is defined by

$$\delta^2(f,\tilde{f}) := \inf_{\tau \in \mathcal{M}} \int \int_{(0,1)^2} |f(\tau(x),\tau(y)) - \tilde{f}(x,y)|^2 \mathrm{d}x\mathrm{d}y$$

$\mathcal{M}$ is the set of all measure-preserving bijections $\tau : [0,1] \to [0,1]$

Property (Lovász 2012)

$\delta(\cdot,\cdot)$ defines a metric on the quotient space $\mathcal{W}$ of graphons.

Minimax rate for sparse SBM in Frobenius norm

K., Tsybakov & Verzelen (2017)

$$\inf_{\widehat{\mathbf{\Theta}}} \sup_{\mathbf{\Theta}_0 \in \mathcal{T}[k,\rho_n]} \mathbb{E}_{\mathbf{\Theta}_0}\left[\frac{1}{n^2}\left\|\widehat{\mathbf{\Theta}} - \mathbf{\Theta}_0\right\|_2^2\right] \asymp \min\left\{\rho_n\left(\frac{\log k}{n} + \frac{k^2}{n^2}\right), \rho_n^2\right\}$$

- $\rho_n = 1$: **Gao et al.(2014)**, the minimax rate over $\mathcal{T}[k,1]$

$$\frac{k^2}{n^2} + \frac{\log k}{n}$$

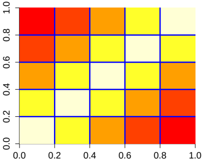
  - $k > \sqrt{n\log(k)}$: nonparametric rate $\dfrac{k^2}{n^2}$
  - $k < \sqrt{n\log(k)}$: clustering rate $\dfrac{\log k}{n}$

From probability matrix estimation to graphon estimation

- To any $n \times n$ probability matrix $\mathbf{\Theta}$ we can associate a graphon.
- Given a $n \times n$ matrix $\mathbf{\Theta}$ with entries in $[0, 1]$, define the **empirical graphon** $\widetilde{f}_{\mathbf{\Theta}}$ as the following piecewise constant function:

$$\widetilde{f}_{\mathbf{\Theta}}(x, y) = \mathbf{\Theta}_{\lceil nx \rceil, \lceil ny \rceil}$$

for all x and y in $(0, 1]$.



- This provides a way of deriving an estimator of the graphon function $f(\cdot, \cdot) = \rho_n W(\cdot, \cdot)$ from **any** estimator of the probability matrix $\mathbf{\Theta}_0$.

From probability matrix estimation to graphon estimation

- **Empirical graphon** $\widetilde{f}_{\mathbf{\Theta}}(x,y) = \mathbf{\Theta}_{\lceil nx\rceil,\lceil ny\rceil}$.
- For any estimator $\widehat{\mathbf{T}}$ of $\mathbf{\Theta}_0$:

$$E\left[\delta^2(\widetilde{f}_{\widehat{\mathbf{T}}}, f)\right] \le 2E\left[\frac{1}{n^2}\|\widehat{\mathbf{T}} - \mathbf{\Theta}_0\|_F^2\right] + 2\underbrace{E\left[\delta^2\left(\widetilde{f}_{\mathbf{\Theta}_0}, f\right)\right]}_{\textbf{agnostic error}}$$

(from the triangle inequality). Here, $\widetilde{f}_{\widehat{\mathbf{T}}}$ and $\widetilde{f}_{\mathbf{\Theta}_0}$ are empirical graphons.

Bound for the δ-risk of step-function graphon

Step function graphons: For some $k \times k$ symmetric matrix $\mathbf{Q}$ and some $\phi : [0,1] \to [k]$,

$$W(x,y) = \mathbf{Q}_{\phi(x),\phi(y)} \quad \text{for all } x, y \in [0,1] \; .$$

Theorem (K., Tsybakov and Verzelen, 2017)

Consider the ρ_n-sparse step-function graphon model W in $\mathcal{W}[k]$. The restricted LS empirical graphon estimator $\widehat{f}$ satisfies

$$E\left[\delta^2\left(\widehat{f}, f\right)\right] \leq C\left[\rho_n\left(\frac{k^2}{n^2} + \frac{\log(k)}{n}\right) + \rho_{\mathbf{n}}^{\mathbf{2}}\sqrt{\frac{\mathbf{k}}{\mathbf{n}}}\right].$$

Sparse network estimation problem

- The optimal rates can be achieved by the Least Squares Estimator
- But: it is not realizable in polynomial time
- Possible gap between the minimax optimal rate and the best rate achievable by computationally feasible methods?
- **Hard thresholding estimator**

Hard thresholding estimator

- **Achieves the best known rate in Frobenius distance in the class of polynomial-time estimators**
- Singular value decomposition of $\mathbf{A}$:

$$\mathbf{A} = \sum_{j=1}^{\mathrm{rank}(\mathbf{A})} \sigma_j(\mathbf{A}) u_j(\mathbf{A}) v_j(\mathbf{A})^T$$

- Tuning parameter $\lambda > 0$:

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

Singular value hard thresholding estimator of Θ_0.

Hard thresholding estimator for sparse SBM

Theorem (K. & Verzelen, 2018)

With high probability

$$\frac{1}{n}\|\widetilde{\mathbf{\Theta}}_\lambda - \mathbf{\Theta}_0\|_2 \;\; \leq \;\; C\sqrt{\frac{\rho_n \mathbf{k}}{n}} \; ,$$

where C is a numerical constant.

- Also minimax optimal in the **cut distance**

- **Cut distance:**
  - Two random graphs with the same edge density are close
  - Reflects global and local structural similarities
  - Cornerstone in the limit graphs theory (**Lovász and Szegedy (2004), Borgs et al (2008), (2012)**):
    - ★ Every graph limit can be represented by a **graphon**
    - ★ A sequence $(\mathcal{G}_n)$ of simple graphs is convergent if and only if it is a Cauchy sequence in the **cut metric**.
- Estimating well the graphon W_0 in the cut distance allows to estimate well the number of small patterns induced by W_0

Matrix cut norm

Matrix cut norm (Frieze and Kannan (1999)):

Matrix $\mathbf{A} = (A_{ij}) \in \mathbb{R}^{n \times n}$

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

- $S = T$, $S \cap T = \emptyset$ or $T = \bar{S}$
- $$\|\mathbf{A}\|_{\square} \leq \frac{1}{n^2} \|\mathbf{A}\|_1 \leq \frac{1}{n} \|\mathbf{A}\|_2$$

where $\|\mathbf{A}\|_1 = \sum_{i,j} |A_{ij}|$ and $\|\mathbf{A}\|_2 = \sqrt{\sum_{i,j} A_{ij}^2}$

Cut norm of graphons

Cut norm of graphons

$$\|W\|_\square = \sup_{S,T\subset[0,1]} \left| \int_{S\times T} W(x,y)\mathrm{d}x\mathrm{d}y \right|$$

- S and T measurable subsets
- $S = T$, $S \cap T = \emptyset$ or $T = \bar{S}$
- $\|W\|_\square \leq \|W\|_1 \leq \|W\|_2 \leq \|W\|_\infty \leq 1$

Minimax rate for sparse SBM in cut norm K. & Verzelen, 2018

$$\inf_{\widehat{\mathbf{\Theta}}} \sup_{\mathbf{\Theta}_0 \in \mathcal{T}[k,\rho_n]} \mathbb{E}_{\mathbf{\Theta}_0}\left[\left\|\widehat{\mathbf{\Theta}} - \mathbf{\Theta}_0\right\|_{\square}\right] \asymp \min\left(\sqrt{\frac{\rho_n}{n}}, \rho_n\right)$$

- Faster than the minimax rate of convergence in Frobenius norm:

$$\inf_{\widehat{\mathbf{\Theta}}} \sup_{\mathbf{\Theta}_0 \in \mathcal{T}[k,\rho_n]} \mathbb{E}_{\mathbf{\Theta}_0}\left[\frac{1}{n}\|\widehat{\mathbf{\Theta}} - \mathbf{\Theta}_0\|_2\right] \asymp \min\left\{\left(\sqrt{\frac{\rho_n \log k}{n}} + \frac{\sqrt{\rho_n} k}{n}\right), \rho_n\right\}$$

  - **Few blocks** $k \lesssim \sqrt{n}$: gain of $\log(k)$ factor
  - **Large** $k \gtrsim \sqrt{n}$: gain of $k/\sqrt{n}$ factor

Graphon estimation problem: step-function graphon

Thresholding empirical graphon estimator

$$\mathbb{E}_W \left[\delta_{\square} \left(\widetilde{f}_{\widetilde{\mathbf{\Theta}}_\lambda}, f_0 \right) \right] \leq C \left(\rho_n \sqrt{\frac{k}{n \log(k)}} + \sqrt{\frac{\rho_n}{n}} \right)$$

- Empirical graphon associated to the hard thresholding estimator is minimax optimal in the cut-distance.
- Achieves best known convergence rates with respect to δ_1 and δ_2-distance among polynomial time algorithms.

Link Prediction

Link prediction

- Networks are often **incomplete**: detecting interactions can require significant experimental effort
- Replace exhaustive testing for every connection by deducing the pairs of nodes which are most likely to interact
- Predict the probabilities of connections from partial observation of the graph

Maximum Likelihood Estimator

- **Wolfe and Olhede (2013)**, **Bickel et al (2013)**, **Amini et al (2013)**, **Celisse et al (2012)** , **Tabouy et al (2017)** ...
- Also NP hard ...
- Computationally efficient approximations:
  - Pseudo-likelihood methods
  - Variational approximation
- Quite successful in practice

Is MLE minimax optimal?

Convergence rate for the MLE

The conditional log-likelihood:

$$\mathcal{L}(\mathbf{A};\mathbf{\Theta}) = \sum_{i<j} \mathbf{A}_{ij}\log(\mathbf{\Theta}_{ij}) + (1-\mathbf{A}_{ij})\log(1-\mathbf{\Theta}_{ij})$$

Theorem (Gaucher & K., 2019)

With high probability

$$\|\mathbf{\Theta}_0 - \widehat{\mathbf{\Theta}}_{ML}\|_2^2 \leq C\rho_n\left(\mathcal{K}(\mathbf{\Theta}_0,\widetilde{\mathbf{\Theta}}) + \frac{\rho_n^2}{(1-\rho_n)^2\wedge\gamma_n^2}\left(k^2+n\log(k)\right)\right).$$

- $0<\gamma_n\leq(\mathbf{\Theta}_0)_{ij}\leq\rho_n<1$
- $\widetilde{\mathbf{\Theta}}$ the best approximation among SBM to $\mathbf{\Theta}_0$ in the sense of the Kullback Leibler divergence
- **Minimax optimal** if $\gamma_n \asymp \rho_n$

Partial observations of the network

- $\mathbf{X} \in \{0,1\}^{n\times n}_{sym}$ **the sampling matrix**:

  $\mathbf{X}_{ij} = 1$ if we observe $\mathbf{A}_{ij}$ and $\mathbf{X}_{ij} = 0$ otherwise
- Conditionally on $\mathbf{\Theta}_0$, $\mathbf{X}$ is independent from the adjacency matrix $\mathbf{A}$
- $\mathbf{X}_{ij}$ are mutually independent
- $\mathbf{\Pi} \in [0,1]^{n\times n}_{sym}$ the **matrix of sampling probabilities**:

  $\mathbf{X}_{ij} \overset{ind.}{\sim}$ Bernoulli$(\mathbf{\Pi}_{ij})$

Partial observations of the network

Particular cases:

- node-based sampling schemes (e.g. the exo-centered design)
- random dyad sampling schemes
- ...

MLE with missing observations

The conditional log-likelihood:

$$\mathcal{L}_{\mathbf{X}}(\mathbf{A};\boldsymbol{\Theta}) = \sum_{i<j} \mathbf{X}_{ij}\left(\mathbf{A}_{ij}\log(\boldsymbol{\Theta}_{ij}) + (1-\mathbf{A}_{ij})\log(1-\boldsymbol{\Theta}_{ij})\right).$$

Theorem (Gaucher & K., 2019)

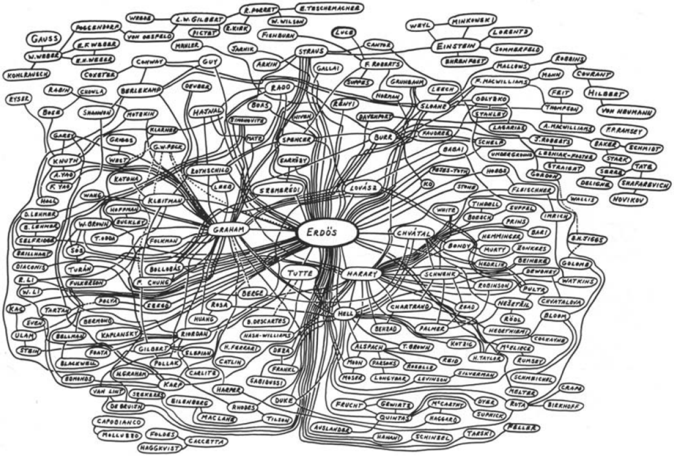
With high probability

$$\|\boldsymbol{\Theta}_0 - \widehat{\boldsymbol{\Theta}}\|^2_{2,\boldsymbol{\Pi}} \leq C'\rho_n\left(\mathcal{K}_{\boldsymbol{\Pi}}(\boldsymbol{\Theta}_0, \widetilde{\boldsymbol{\Theta}}) + \frac{\rho_n^2}{(1-\rho_n)^2 \wedge \gamma_n^2}\left(k^2 + n\log(k)\right)\right).$$

- $\|\boldsymbol{\Theta}_0 - \widehat{\boldsymbol{\Theta}}\|^2_{2,\boldsymbol{\Pi}} = \sum_{ij} \boldsymbol{\Pi}_{ij}(\boldsymbol{\Theta}_0 - \widehat{\boldsymbol{\Theta}})^2_{ij}$
- **Minimax optimal** if $c_1 p \leq \boldsymbol{\Pi}_{ij} \leq c_2 p$ [**Gao et al, 2016**]

Conclusion

- **Least Squares Estimator**:
  - attains the optimal rates in a minimax sense,
  - not realizable in polynomial time
- better choice: **Thresholding estimator** (slower rates of convergence)
- **MLE:**
  - minimax optimal
  - has computationally efficient approximations
- **Link Prediction:**
  - MLE: enables rank unobserved pairs of nodes
  - Minimax optimality of this approach
  - Works for quite general sampling schemes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RUMSEY
COCKAYNE

Thank You !