

Uniform estimation of some random graph parameters

Ismaël Castillo

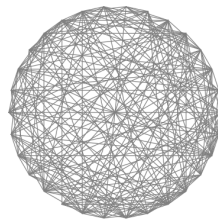
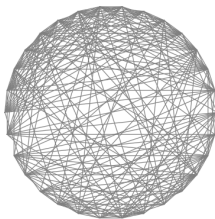
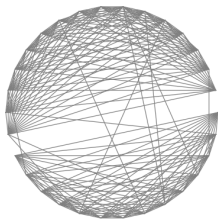
LPMA – Université Paris VI

joint work with Peter Orbanz (Columbia)

Mathematical Methods of Statistics
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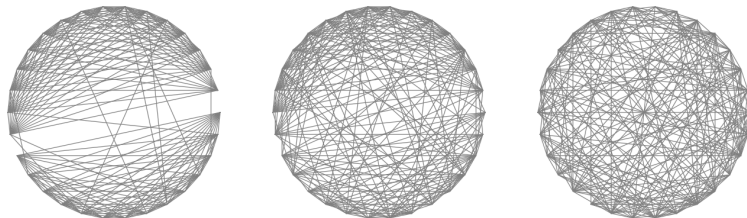
Random graph models

Graph samples with $n = 30$ nodes



Random graph models

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How does the *information* grow with n ?

Random graph models

- Given a probability model for the random graph [next slides]

$$\mathcal{P} = \{P_{\eta}^{(n)}, \eta \in H\}$$

Collection of possible distributions for $(X_{ij})_{1 \leq i < j \leq n}$, where

- $X_{ij} \in \{0, 1\}$ tells whether an edge is present or not between nodes i and j
- One may be interested in estimation of
 - the 'parameters' η
 - and/or of functionals $\psi(P_{\eta})$ of those
- Example: edge density $E_{P_{\eta}}[X_{ij}]$
 - Possible estimator

$$\frac{1}{\binom{n}{2}} \sum_{i < j} X_{ij}$$

Random graph models: SBM

The *stochastic block model* SBM with K classes

- Parameters

- ▶ $p = (p_1, \dots, p_K)$ prob. of classes
- ▶ $Q = (Q_{kl})$ symmetric $K \times K$ matrix prob. of connection between classes

- Notation: labels

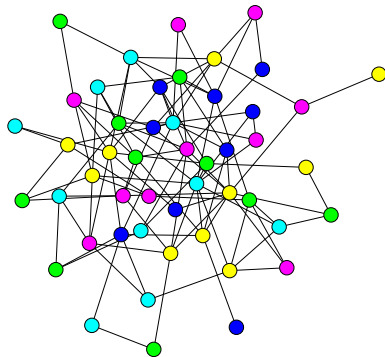
- ▶ $\varphi : \{1, \dots, n\} \rightarrow \{1, \dots, K\}$ assigns a class to each vertex

- Observations: $(X_{ij})_{i < j}$ [the labelling map φ is **not** observed]

Let $\pi = p_1 \delta_1 + \dots + p_K \delta_K$. The data distribution is

$$\begin{aligned}(\varphi(1), \dots, \varphi(n)) &\sim \pi^{\otimes n}, \\(X_{ij})_{i < j} \mid \varphi &\sim \bigotimes_{i < j} \text{Be}(Q_{\varphi(i)\varphi(j)})\end{aligned}$$

Random graph models: SBM



- $K = 5$
- $p = (p_1, \dots, p_5)$
probabilities of classes
- Q a 5×5 matrix of connectivities

Random graph models: graphon model

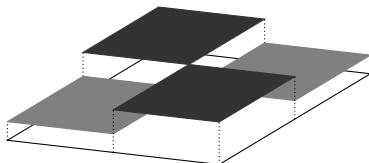
The *graphon model*

- Parameter
 - ▶ $f : [0, 1]^2 \rightarrow [0, 1]$ measurable symmetric
- Observations: $(X_{ij})_{i < j}$ [the design variables U_i are **not** observed]

$$\begin{aligned}(U_i)_i &\sim \text{Unif}[0, 1]^{\otimes n} \\ (X_{ij})_{i < j} \mid (U_i)_i &\sim \bigotimes_{i < j} \text{Be}(f(U_i, U_j))\end{aligned}$$

Random graph models

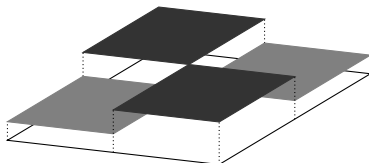
- The SBM model as a graphon model



$\frac{1}{2} + \theta$	$\frac{1}{2} - \theta$
$\frac{1}{2} - \theta$	$\frac{1}{2} + \theta$

Random graph models

- The SBM model as a graphon model



$\frac{1}{2} + \theta$	$\frac{1}{2} - \theta$
$\frac{1}{2} - \theta$	$\frac{1}{2} + \theta$

- Matrix $Q = (Q_{ij})$ of SBM model can be read as **heights** of histogram with partition on $[0, 1]$ given by **proportions** vector p

SBM: estimation of parameters

[Bickel et al 2013]

[here in case $\mathbb{P}[X_{ij} = 1] =: \rho \sim \text{cst.}$]

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- Assume that
 - ▶ $K = K_0$ is known and fixed
 - ▶ no two lines of matrix Q_0 are the same and $\min_k p_{0,k} \neq 0$
- First, what happens if labels $\varphi(\cdot)$ would be **observed**?

SBM: estimation of parameters

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- First, what happens if labels $\varphi(\cdot)$ would be **observed**?
 - ▶ the MLE $(\tilde{p}^{ML}, \tilde{Q}^{ML})$ is asymptotically normal

$$\sqrt{n}(\tilde{p}^{ML} - p_0) \mid \varphi \rightarrow \mathcal{N}(0, T_1)$$

$$n(\tilde{Q}^{ML} - Q_0) \mid \varphi \rightarrow \mathcal{N}(0, T_2)$$

$$\tilde{p}_a^{ML} = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\varphi(i)=a}, \quad \tilde{Q}_{ab}^{ML} = \frac{\sum_{i < j} X_{ij} \mathbb{1}_{\varphi(i)=a, \varphi(j)=b}}{\sum_{i < j} \mathbb{1}_{\varphi(i)=a, \varphi(j)=b}}$$

SBM: estimation of parameters

[Bickel et al 2013]

- **Theorem.** If labels are **unknown**, under the previous assumptions
 - ▶ the MLE $(\hat{p}^{ML}, \hat{Q}^{ML})$ is asymptotically normal

$$\sqrt{n}(\hat{p}^{ML*} - p_0) \rightarrow \mathcal{N}(0, T_1)$$

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where (p^*, Q^*) denotes a label switched-version of (p, Q)

SBM: estimation of parameters

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- *Pointwise* inference is *asymptotically* equivalent to given φ case

- ▶ Idea : ML 'profiles out' the unknown φ
→ proof based on $\hat{\varphi}$ that consistently estimates φ asymptotically

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- Note that

- ▶ p_0 estimated at 'slow' rate $\frac{1}{\sqrt{n}} \rightarrow \frac{1}{n}$ in terms of quadratic risk
- ▶ Q_0 estimated at 'fast' rate $\frac{1}{n} \rightarrow \frac{1}{n^2}$ in terms of quadratic risk

Some questions

The previous results are *asymptotic* and *pointwise* at (p_0, Q_0)

Some questions

- *uniform* estimation of parameters?
→ say of the **connectivity** parameters = the matrix Q
- in practice n and K are free
→ non-asymptotic results where K is possibly 'large'?

Framework : **SBM** (to start with)

Related topics

- Testing and ‘community’ detection
[Arias-Castro, Candès and Durand 2011]
[Butucea and Ingster 2013]
[Arias-Castro and Verzelen 2014-15]
- Estimation of the graphon function f [wrt squared L^2 -type risk]
[Olhede and Wolfe 2013]
[Gao, Lu and Zhou 2015]
[Klopp, Tsybakov and Verzelen 2015]
- Other random graph models
‘sparsified’ graphon model, preferential attachment, graphex model, ...

A first result $K = 2$

For simplicity assume equiproportions $p_1 = p_2 = \frac{1}{2}$

- Consider the SBM submodel $p = [\frac{1}{2}, \frac{1}{2}]$, $Q = Q^\theta$, $K = 2$, with

$$Q^\theta = \begin{bmatrix} \frac{1}{2} + \theta & \frac{1}{2} - \theta \\ \frac{1}{2} - \theta & \frac{1}{2} + \theta \end{bmatrix}$$

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- Theorem 1** [*minimax lower bound*]. For some $c_0 > 0$,

$$\inf_{\hat{\theta}} \sup_{|\theta| \leq \frac{1}{2}} E_{\theta} \left[(\hat{\theta} - \theta)^2 \right] \geq \frac{c_0}{n}.$$

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- ▶ minimax **local** lower bound, relevant not only at $\theta = 0$, but also locally

can show that if $t = \frac{\delta_0}{2n}$,

$$\inf_{\hat{\theta}} \sup_{|\theta - t| < \frac{\delta_0}{2n}} E_\theta \left[(\hat{\theta} - \theta)^2 \right] \geq \frac{c_0}{n}.$$

A first result $K=2$

- Consider the submodel

$$Q^\theta = \begin{bmatrix} \frac{1}{2} + \theta & \frac{1}{2} - \theta \\ \frac{1}{2} - \theta & \frac{1}{2} + \theta \end{bmatrix}$$

One observes SBM-data with $p = [\frac{1}{2}, \frac{1}{2}]$, $Q = Q^\theta$, $K = 2$

- Let $\hat{\theta}^{ML}$ be the MLE in the above submodel
- Theorem** 1 (bis) [*minimax upper bound*]. For some $d_0 > 0$,

$$\sup_{|\theta| \leq \frac{1}{2}} E_\theta \left[(\hat{\theta}^{ML} - \theta)^2 \right] \leq \frac{d_0}{n}$$

Proof: profile (pseudo)-maximum likelihood

Main result for $K = k$ classes, motivation

An example with $n = 30$, $K = 5$ and a 'difficult' matrix Q

$$\begin{bmatrix} .55 & .45 & .4 & .1 & .7 \\ .45 & .55 & .4 & .1 & .7 \\ .4 & .4 & .6 & .2 & .1 \\ .1 & .1 & .2 & .1 & .4 \\ .7 & .7 & .4 & .4 & .2 \end{bmatrix}$$

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Local uniform estimation rate of elements of **this** submatrix will be 'slow'

SBM result $K = k$ classes

Suppose equiproportions for simplicity [balanced proportions would work]

Let us consider estimation along the submodel

$$\begin{bmatrix} a_0 & a_1 & \dots & a_{k-2} \\ a_1 & & & \\ \vdots & & B & \\ a_{k-2} & & & \end{bmatrix}$$

SBM result $K = k$ classes

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Let us consider estimation along the submodel

$$\begin{bmatrix} a_0 & a_1 & \cdots & a_{k-2} \\ a_1 & & & \\ \vdots & & B & \\ a_{k-2} & & & \end{bmatrix} \rightarrow \begin{bmatrix} a_0 + \theta & a_0 - \theta & a_1 & \cdots & a_{k-2} \\ a_0 - \theta & a_0 + \theta & a_1 & \cdots & a_{k-2} \\ a_1 & a_1 & & & \\ \vdots & \vdots & & B & \\ a_{k-2} & a_{k-2} & & & \end{bmatrix} = Q^\theta$$

Set $A = [a_0 \ a_1 \ \cdots \ a_{k-2}]$ and $B = (b_{ij})$

SBM result $K = k$ classes

Suppose proportions are equidistributed [extends to 'balanced proportions']

- main message of Theorem 2 below

Around *any* point in the interior of the $K = k - 1$ classes model,
there is a direction coming from the $K = k$ classes model such that
rate of estimation of matrix parameter along this direction no better than $\frac{k}{n}$

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- One observes SBM-data with law E_θ specified by

$$K = k, \quad p = \left[\frac{1}{K}, \dots, \frac{1}{K} \right], \quad Q = Q^\theta \text{ the previous } K \times K \text{ matrix}$$

- **Theorem 2** [*minimax lower bound*]. For some $c_1 > 0$, for *any* A and B ,

$$\inf_{\hat{\theta}} \sup_{|\theta| \leq \frac{1}{2}} E_\theta \left[(\hat{\theta} - \theta)^2 \right] \geq c_1 \frac{k}{n}.$$

Comments on the lower bound

- The bound is minimax *local*
- Idea of proof of lower bound
 - a 'mixture vs mixture' lower bound argument
 - more involved than before, as 'null hypothesis' is a mixture

SBM result $K = k$ classes

Implications

- The 'boundary' of SBM model with $K = k$ moves with k and n
- If one is interested in estimating (some of the) heights = elements of the Q matrix, one should take this moving boundary into account to determine precisely the accuracy of estimation
- The rate along constructed submodel deteriorates with k .

The lower bound is non-asymptotic.

For many k, n , the boundary area, of size at least $\frac{k}{n}$, can be 'large'

Upper-bound result

Recall

$$Q^\theta = \begin{bmatrix} a_0 + \theta & a_0 - \theta & a_1 & \dots & a_{k-2} \\ a_0 - \theta & a_0 + \theta & a_1 & \dots & a_{k-2} \\ a_1 & a_1 & & & \\ \vdots & \vdots & & & \\ a_{k-2} & a_{k-2} & & & \end{bmatrix} \quad B = (b_{ij})$$

- Require, for $\mathcal{C} := \{a_i, b_{ij}, 1 \leq i, j \leq k-2\}$,

$$\min_{c \in \mathcal{C}} \{|c - a_0|\} \geq \kappa > 0 \quad (C)$$

$$k^3 \log k \lesssim \kappa^4 n \quad (D)$$

Upper-bound result

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$$Q^\theta = \begin{bmatrix} a_0 + \theta & a_0 - \theta & a_1 & \dots & a_{k-2} \\ a_0 - \theta & a_0 + \theta & a_1 & \dots & a_{k-2} \\ a_1 & a_1 & & & \\ \vdots & \vdots & & & \\ a_{k-2} & a_{k-2} & & & \end{bmatrix} \quad B = (b_{ij})$$

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- Theorem 3** [upper bound]. For some $C_1 > 0$, for any A, B such that conditions (C)–(D) hold, for $\hat{\theta}$ a profile-MLE estimate,

$$\sup_{|\theta| \leq \kappa} E_\theta \left[(\hat{\theta} - \theta)^2 \right] \leq C_1 \frac{k}{n}.$$

Upper-bound result – checking (C) and (D)

Conditions (C) and (D) are satisfied in the following settings

- *Example 1 (well-separated block)*

If κ is a given positive constant e.g. $\kappa = 1/4$, then (C) means that the coefficients of A, B are fairly different from a_0

- *Example 2 (randomly sampled matrices A, B)*

If the vector defining A and the upper half of the matrix B are sampled iid $\mathcal{U}[0, 1]$, then (C)-(D) is satisfied with high probability if

$$k \lesssim n^{1/7}$$

Dependence on the 'environment' A and B

Consider a 'least-favorable case'

$$Z^\theta = \begin{bmatrix} \frac{1}{2} + \theta & \frac{1}{2} - \theta & \frac{1}{2} & \cdots & \frac{1}{2} \\ \frac{1}{2} - \theta & \frac{1}{2} + \theta & \frac{1}{2} & \cdots & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \cdots & \frac{1}{2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \cdots & \frac{1}{2} \end{bmatrix}.$$

[or a perturbation thereof]

Observe data from the corresponding SBM model with equiproportions

- **Theorem 4.** There exists $c_2 > 0$ such that

$$\inf_{\hat{\theta}} \sup_{\theta \in (-1/2, 1/2)} E_\theta(\hat{\theta} - \theta)^2 \geq c_2 \frac{k^2}{n}$$

Functionals of graphon model

In the more general graphon model, consider the functional

$$\psi(\langle f \rangle) = \left[\int_{[0,1]^2} \left(f(x,y) - \int_{[0,1]^2} f \right)^2 dx dy \right]^{1/2}$$

[Continuous ‘graphon-analogue’ of previous parameter θ]

- **Theorem** 5. For $\mathcal{P}$ a $\mathcal{C}^1(M)$ -class of graphons, for some $c_3, c_4 > 0$,

$$\frac{c_3}{n} \leq \inf_{\hat{\psi}} \sup_{f \in \mathcal{P}} E_f \left[(\hat{\psi} - \psi(f))^2 \right] \leq \frac{c_4}{n}.$$

Functionals of graphon model

- Lower bound also holds for other functionals such as

$$\psi(P_w) = \int_{[0,1]^2} \left| f(x, y) - \int_{[0,1]^2} |f(x, y)| dx dy \right| dx dy$$

- The quadratic ‘slow rate’ $1/n$ [or $1/\sqrt{n}$ non-quadratic] appears to be quite universal for uniform estimation of many functionals

Conclusion

Previously known results for SBMs (K, p, Q) : given fixed $K = k$,

- proportions p estimated at 'slow' rate $\frac{1}{n}$ asymptotically
- connectivities Q estimated at 'fast' rate $\frac{1}{n^2}$ asymptotically,
pointwise, in the *interior* of set of SBMs with k classes

Conclusions

- Fast rate for connectivities Q not achievable uniformly

Uniform rates are at most k/n [=generic lower bound if k not too large] and can be as slow as k^2/n , from a non-asymptotic perspective in n and k

- This phenomenon happens close to *any* $k - 1$ classes model, not only around a 'least favorable one' → local lower bound

Open questions

- SBM: 'Continuum' of rates inbetween k/n and k^2/n depending on A, B ?
- More general estimation theory of graphon functionals?