

Sparse Network Estimation

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Joint works with



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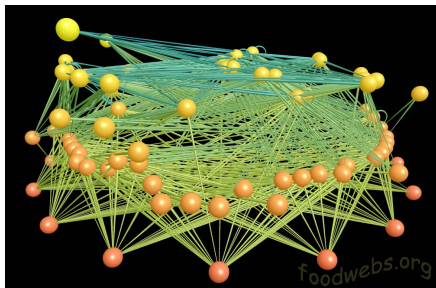


Nicolas Verzelen



Solenne Gaucher

Network model



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

Approach

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

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 $\{C_1, \dots, C_k\}$
 - ▶ each node i is associated with a community $z(i)$
 - ▶ $z : [n] \rightarrow [k]$: the index function
 - ▶ z : a parameter to estimate (the conditional SBM), or a latent variable
 - ▶ 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.

Inhomogeneous random graph model

- ▶ We observe the $n \times n$ adjacency matrix $\mathbf{A} = (A_{ij})$ of a graph
- ▶ A_{ij} are Bernoulli random variables with parameter Θ_{ij}
- ▶ Θ_0 is the $n \times n$ symmetric matrix with entries (Θ_{ij}) (the matrix of probabilities associated to the graph)
 - ▶ vertices i and j are connected by an edge with probability Θ_{ij} independently from any other edge
 - ▶ sparsity parameter $\rho_n = \max_{ij} \Theta_{ij} \rightarrow 0$ and $\rho_n \geq 1/n$
- ▶ Given a single observation \mathbf{A} , we want to estimate Θ_0

Minimax rate for sparse SBM in Frobenius norm

The best rate of convergence that any estimator may achieve:

K., Tsybakov & Verzelen (2017)

$$\inf_{\hat{\Theta}} \sup_{\Theta_0 \in \mathcal{T}[k, \rho_n]} \mathbb{E}_{\Theta_0} \left[\frac{1}{n^2} \left\| \hat{\Theta} - \Theta_0 \right\|_2^2 \right] \asymp \min \left\{ \rho_n \left(\frac{\log k}{n} + \frac{k^2}{n^2} \right), \rho_n^2 \right\}$$

- ▶ $\rho_n = 1$: **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 $\frac{k^2}{n^2}$
- ▶ $k < \sqrt{n \log(k)}$: clustering rate $\frac{\log k}{n}$

Sparse network estimation problem

- ▶ The optimal rates can be achieved by the **Least Squares Estimator**
- ▶ But: not realizable in polynomial time
- ▶ Better choices:
 - ▶ Maximum Likelihood Estimator
 - ▶ Hard thresholding estimator
 - ▶ ...

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:

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

The maximum log-likelihood estimator of Θ^* :

$$(\hat{\mathbf{Q}}, \hat{z}) \in \underset{Q \in [0,1]^{k \times k}, z \in \mathcal{Z}_{n,k}}{\operatorname{argmax}} \mathcal{L}(\mathbf{A}; z, \mathbf{Q}).$$

$\mathcal{Z}_{n,k}$ the set of all possible mappings z from $[n]$ to $[k]$

Theorem (Gaucher & K., 2021)

With high probability

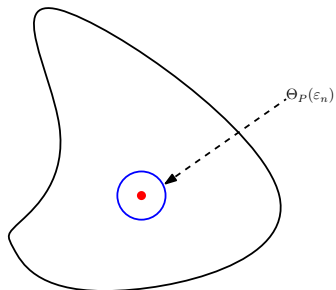
$$\frac{1}{n^2} \|\Theta_0 - \hat{\Theta}_{ML}\|_2^2 \leq C_{\rho_n, \gamma_n} \rho_n \left(\frac{\log k}{n} + \frac{k^2}{n^2} \right).$$

- ▶ $0 < \gamma_n \leq \Theta_{ij} \leq \rho_n < 1$
- ▶ **Minimax optimal** if $\gamma_n \asymp \rho_n$

Variational approximation

- ▶ The optimization of the likelihood function requires a search over the set of k^n labels \Rightarrow MLE is computationally intractable
- ▶ Solution: **Variational approximation**
 - ▶ serves to approximate the posterior
 - ▶ distributions for the unobserved variables (parameters, latent variables)
 - ▶ often hard-to-solve integrals
 - ▶ Kullback–Leibler divergency as a measure of good approximation
 - ▶ Assuming the unknown variables can be partitioned so that each partition is independent: **the mean-field approximation**
 - ▶ Often results in easy to compute interactive algorithms

Subhabrata's talk: variational approximation can lead to a quite accurate approximation



S. Sen's courtesy

The mean field approximation works exceptionally well for the SBM

Variational approximation to the MLE

- ▶ [Celisse et al \(2008\)](#) and [Bickel et al \(2013\)](#): variational approximation
 - ▶ asymptotic normality for variational methods for parameter estimates of stochastic block data
- ▶ The problem of community detection: [Edoardo et al \(2008\)](#), [Hofman et al \(2008\)](#), [Zhang et al \(2020\)](#), [Razaei et al \(2019\)](#)
...
- ▶ [Gaucher & K. \(2021\)](#):
 - ▶ optimal statistical accuracy
 - ▶ labels recovery

SBM with random labels

- ▶ Nodes are classified into k communities:
 - ▶ each node i is associated with a community $z(i)$
 - ▶ $z : [n] \rightarrow [k]$: the index function
 - ▶ z : a parameter to estimate (the conditional SBM), or a latent variable
- ▶ **The indexes follow a multinomial distribution:**

$$\forall i \quad z(i) \stackrel{i.i.d}{\sim} \mathcal{M}(1; \alpha)$$

- ▶ $\forall l \in [k]$, α_l is the probability that node i belongs to the community l
 - ▶ $\alpha_k n$ is the expected size of community k
 - ▶ the probabilities of connection are given by a $k \times k$ matrix \mathbf{Q}
- ▶ We consider a SBM with parameters (α, \mathbf{Q}) .

Variational approximation to the MLE

- ▶ SBM with parameters (α, \mathbf{Q})
- ▶ The likelihood of the observed adjacency matrix \mathbf{A} :

$$l(\mathbf{A}; \alpha, \mathbf{Q}) = \sum_{z \in \mathcal{Z}_{n,k}} \left(\prod_{i \leq n} \alpha_{z(i)} \right) \exp(\mathcal{L}(\mathbf{A}; z, \mathbf{Q})).$$

- ▶ the maximization still requires to evaluate the expectation of the label function z by summing over k^n possible labels
- ▶ Solution: use the **mean-field approximation**

Mean-field approximation

$$l(\mathbf{A}; \alpha, \mathbf{Q}) = \sum_{z \in \mathcal{Z}_{n,k}} \left(\prod_{i \leq n} \alpha_{z(i)} \right) \exp(\mathcal{L}(\mathbf{A}; z, \mathbf{Q})).$$

- ▶ Approximate the posterior distribution of z by a simpler distribution:
 - ▶ the posterior distribution $\mathbb{P}(\cdot | \mathbf{A}, \alpha, \mathbf{Q})$ is approximated by a multinomial distribution \mathbb{P}_τ , s.t. $\mathbb{P}_\tau(z) = \prod_{1 \leq i \leq n} \mathcal{M}(z | \tau^i)$
 - ▶ $\tau^i = (\tau_1^i, \dots, \tau_K^i)$
 - ▶ $\tau = (\tau^1, \dots, \tau^n)$
- ▶ Use the KL-divergence as a measure of how well our approximation fits the true posterior

Variational approximation to the MLE

The variational estimator:

$$\left(\hat{\alpha}^{VAR}, \hat{\mathbf{Q}}^{VAR}, \hat{\tau}^{VAR}\right) = \underset{\alpha \in \mathcal{A}, \mathbf{Q} \in \mathcal{Q}, \tau \in \mathcal{T}}{\operatorname{argmax}} \mathcal{J}(\mathbf{A}; \tau, \alpha, \mathbf{Q}) \quad (1)$$

for $\mathcal{J}(\mathbf{A}; \tau, \alpha, \mathbf{Q}) = \mathfrak{l}(\mathbf{A}; \alpha, \mathbf{Q}) - KL(\mathbb{P}_{\tau}(\cdot) || \mathbb{P}(\cdot | \mathbf{A}, \alpha, \mathbf{Q}))$

- ▶ \mathcal{A} , \mathcal{Q} and \mathcal{T} : the parameter spaces for the parameters α , \mathbf{Q} and τ
- ▶ KL : the Kullback-Leibler divergence
- ▶ $\mathcal{J}(\mathbf{A}; \tau, \alpha, \mathbf{Q})$ provides a lower bound on $\mathfrak{l}(\mathbf{A}; \alpha, \mathbf{Q})$

EM algorithm

The expectation - maximization (EM) algorithm [Tabouy et al \(2020\)](#):

- ▶ Estimation Step: given parameters (α, \mathbf{Q}) , the variational parameter τ maximizing $\mathcal{J}(\mathbf{A}; \tau, \alpha, \mathbf{Q})$ is given by the fixed point equation :

$$\tau_k^i \propto \alpha_k \prod_{j \neq i} \prod_{l \leq K} \left(\mathbf{Q}_{kl}^{\mathbf{A}_{ij}} (1 - \mathbf{Q}_{kl})^{1 - \mathbf{A}_{ij}} \right)^{\tau_l^j};$$

- ▶ Maximisation Step: given parameter τ , the parameters (α, \mathbf{Q}) maximizing $\mathcal{J}(\mathbf{A}; \tau, \alpha, \mathbf{Q})$ are given by

$$\alpha_k = \frac{\sum_i \tau_k^i}{n}, \quad \mathbf{Q}_{kl} = \frac{\sum_{i \neq j} \tau_k^i \tau_l^j \mathbf{A}_{ij}}{\sum_{i \neq j} \tau_k^i \tau_l^j}.$$

Statistical guarantees for the variational estimator

- ▶ Celisse et al (2008) and Bickel et al (2013):
 - ▶ maximizing $\max_{\tau \in \mathcal{T}} \mathcal{J}(\mathbf{A}; \tau, \alpha, \mathbf{Q})$ is equivalent to maximising $l(\mathbf{A}; \alpha, \mathbf{Q})$
 - ▶ the estimator obtained by maximizing $l(\mathbf{A}; \alpha, \mathbf{Q})$ converges to the true parameters (α, \mathbf{Q})
 - ▶ $(\hat{\alpha}^{VAR}, \hat{\mathbf{Q}}^{VAR})$ also converges to (α, \mathbf{Q})
 - ▶ does not provide guarantees on the recovery of the true labels z

The label estimator

- ▶ The label estimator \hat{z}^{VAR} :

$$\forall i \leq n, \hat{z}^{VAR}(i) \triangleq \operatorname{argmax}_{k \leq K} (\hat{\tau}^{VAR})_k^i$$

- ▶ Replace $\hat{\mathbf{Q}}^{VAR}$ by the empirical mean estimator:

$$\hat{\mathbf{Q}}_{ab}^{ML-VAR} \triangleq \frac{\sum_{i \in (\hat{z}^{VAR})^{-1}(a), j \in (\hat{z}^{VAR})^{-1}(b), i \neq j} \mathbf{A}_{ij}}{n_{ab}}$$



$$n_{ab}(\hat{z}^{VAR}) = \begin{cases} |(\hat{z}^{VAR})^{-1}(a)| \times |(\hat{z}^{VAR})^{-1}(b)| & \text{if } a \neq b \\ |(\hat{z}^{VAR})^{-1}(a)| \times (|(\hat{z}^{VAR})^{-1}(a)| - 1) & \text{otherwise} \end{cases}$$

- ▶ Define $\hat{\Theta}^{VAR}$ as

$$\hat{\Theta}_{i \neq j}^{VAR} = \hat{\mathbf{Q}}_{\hat{z}^{VAR}(i), \hat{z}^{VAR}(j)}^{ML-VAR}, \quad \hat{\Theta}_{ii}^{VAR} = 0.$$

Statistical guarantees for the variational estimator

This new estimator $(\hat{z}^{VAR}, \hat{\mathbf{Q}}^{ML-VAR})$ is minimax optimal:

Theorem (Gaucher & K., 2021)

Assume that \mathbf{Q}^0 has no identical columns and the sparsity inducing sequence ρ_n satisfies $\rho_n \gg \log(n)/n$. Then, there exists a constant $C_{\mathbf{Q}^0} > 0$ depending on \mathbf{Q}^0 such that

$$\mathbb{P}\left(\left\|\Theta_0 - \hat{\Theta}^{VAR}\right\|_2^2 \leq C_{\mathbf{Q}^0} \rho_n (k^2 + n \log(k))\right) \xrightarrow{n \rightarrow \infty} 1$$

1. $\alpha = \alpha^0$ for some fixed α^0 such that $\alpha_a^0 > 0$ for any $a \in \{1, \dots, k\}$
2. $\mathbf{Q} = \rho_n \mathbf{Q}^0$ for some fixed $\mathbf{Q}^0 \in (0, 1)^{k \times k}$ such that

$$\sum_{a,b=1}^k \alpha_a^0 \alpha_b^0 \mathbf{Q}_{ab}^0 = 1$$

How does it work ?

- ▶ Variational approximation to the MLE has been used for estimation of (\mathbf{Q}, α)
- ▶ We show that **both the maximum likelihood estimator and its variational counterpart can perfectly recover all labels**:
 - ▶ with large probability, there exists a permutation σ of $\{1, \dots, K\}$ such that $(\hat{z}^{VAR}(\sigma(k)))_{k \leq K} = (\hat{z}(k))_{k \leq K}$
 - ▶ (under certain conditions) MLE recovers the true labels
- ▶ exact recovery of the labels have already been established in this regime under more restricted assumptions (see [Abbe \(2018\)](#)):
 - ▶ the SBM is symmetric, assortative and has balanced communities

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

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

- ▶ 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:

- ▶ $\xi = (\xi_1, \dots, \xi_n)$ are latent i.i.d. uniformly distributed on $[0, 1]$.

$$\Theta_{ij} = W_0(\xi_i, \xi_j).$$

- ▶ The diagonal entries Θ_{ii} are zero and $\Theta_0 = (\Theta_{ij})$
- ▶ Given Θ_0 the graph is sampled according to the **inhomogeneous random graph model**:
 - ▶ vertices i and j are connected by an edge with probability Θ_{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 $\rho_n \rightarrow 0$ as $n \rightarrow \infty$.
 - ▶ The adjacency matrix \mathbf{A} is sampled according to graphon W_0 with scaling parameter ρ_n :

$$\Theta_{ij} = \rho_n W_0(\xi_i, \xi_j), \quad i < j.$$

- ▶ $\rho_n =$ “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

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

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

\mathcal{M} is the set of all measure-preserving bijections

$$\tau : [0, 1] \rightarrow [0, 1]$$

Property (Lovász 2012)

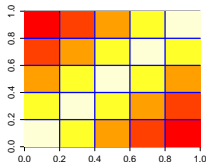
$\delta(\cdot, \cdot)$ defines a metric on the quotient space \mathcal{W} of graphons.

From probability matrix estimation to graphon estimation

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

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

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 Θ_0 .

From probability matrix estimation to graphon estimation

- ▶ **Empirical graphon** $\tilde{f}_{\Theta}(x, y) = \Theta_{\lceil nx \rceil, \lceil ny \rceil}$.
- ▶ For any estimator $\hat{\mathbf{T}}$ of Θ_0 :

$$\mathbb{E} \left[\delta^2(\tilde{f}_{\hat{\mathbf{T}}}, f) \right] \leq 2\mathbb{E} \left[\frac{1}{n^2} \|\hat{\mathbf{T}} - \Theta_0\|_F^2 \right] + \underbrace{2\mathbb{E} \left[\delta^2(\tilde{f}_{\Theta_0}, f) \right]}_{\text{agnostic error}}$$

(from the triangle inequality). Here, $\tilde{f}_{\hat{\mathbf{T}}}$ and \tilde{f}_{Θ_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 $\phi : [0, 1] \rightarrow [k]$,

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

Theorem (K., Tsybakov and Verzelen, 2017)

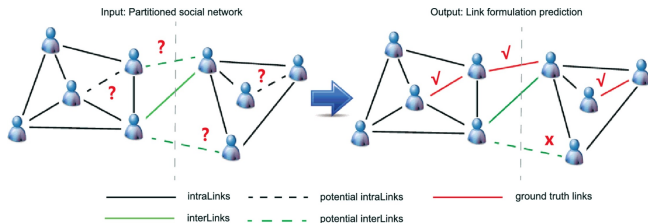
Consider the ρ_n -sparse step-function graphon model $\mathcal{W}[k, \rho_n]$.

$$\inf_{\hat{f}} \sup_{f \in \mathcal{W}[k, \rho_n]} \mathbb{E} \left[\delta^2 \left(\hat{f}, f \right) \right] \asymp \left[\rho_n \left(\frac{k^2}{n^2} + \frac{\log(k)}{n} \right) + \rho_n^2 \sqrt{\frac{k}{n}} \right].$$

Missing Links

Real-life networks are only partially observed

- ▶ Exhaustive exploration of all interactions in a network is expensive
- ▶ Survey data: non-response or drop-out of participants
- ▶ Online social network data: sub-sample of the network



A balanced modularity maximization link prediction model in social networks [Wu et al.(2017)]

Conditional maximum likelihood estimator

- ▶ the log-likelihood function with respect to the observed entries of the adjacency matrix \mathbf{A} and sampling matrix \mathbf{X} :

$$\begin{aligned}\mathcal{L}_{\mathbf{X}}(\mathbf{A}; z, \mathbf{Q}) &= \sum_{1 \leq i < j \leq n} \mathbf{X}_{ij} (\mathbf{A}_{ij} \log(\mathbf{Q}_{z(i)z(j)}) \\ &\quad + (1 - \mathbf{A}_{ij}) \log(1 - \mathbf{Q}_{z(i)z(j)})) \\ &= \sum_{a \leq b} \log(\mathbf{Q}_{ab}) \sum_{\substack{i \in z^{-1}(a), j \in z^{-1}(b) \\ i \neq j}} \mathbf{X}_{ij} \mathbf{A}_{ij} \\ &\quad + \sum_{a \leq b} \log(1 - \mathbf{Q}_{ab}) \sum_{\substack{i \in z^{-1}(a), j \in z^{-1}(b) \\ i \neq j}} \mathbf{X}_{ij} (1 - \mathbf{A}_{ij})\end{aligned}$$

- ▶ X_{ij} are iid Bernoulli (p)

Theorem (Gaucher & K., 2021)

Assume that \mathbf{Q}^0 has no identical columns and the sparsity inducing sequence ρ_n satisfies $\rho_n \gg \log(n)/(pn)$. Then,

$$\mathbb{P}(\hat{z}^{VAR} \sim \hat{z}) \rightarrow 1$$

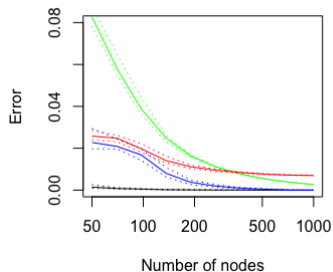
when $n \rightarrow \infty$. Moreover, there exists a constant $C_{\mathbf{Q}^0} > 0$ depending on \mathbf{Q}^0 such that

$$\mathbb{P}\left(\left\|\Theta^* - \hat{\Theta}^{VAR}\right\|_2^2 \leq \frac{C_{\mathbf{Q}^0} (k^2 + n \log(k))}{p}\right) \xrightarrow{n \rightarrow \infty} 1.$$

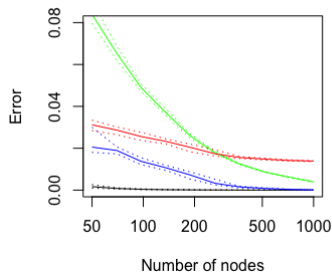
Empirical performances of the variational approximation of MLE

We compare the variational approximation to the MLE to

- ▶ missSBM
- ▶ softImpute
- ▶ the oracle estimator with knowledge of the label z^*

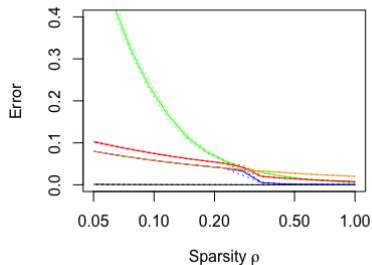


Assortative SBM

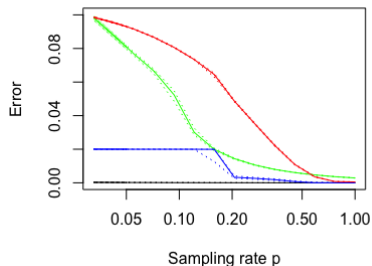


Robustness against sparsity and missing observations

Error of connection probabilities estimation as a function of the sparsity parameter ρ and of the sampling rate p ($n = 500$):



Robustness against sparsity



Robustness against missing observations.

Interactions within a elementary school

- ▶ Network of interactions within a French elementary school Stehle et al (2011) :
 - ▶ Physical interactions between 222 children divided into 10 classes and their 10 teachers
 - ▶ Two consecutive days
 - ▶ Homogeneous degrees (the maximum degree is 41, the minimum degree is 5 and the mean degree is 20)
 - ▶ Strong community structure. Therefore, we expect the networks of interactions to be well approximated by a stochastic block model
- ▶ Two outcomes of the same random network model:
 - ▶ We use the observations collected on Day 1 to estimate the matrix Θ^*
 - ▶ Evaluate the estimators on the network of Day 2

Interactions within a elementary school

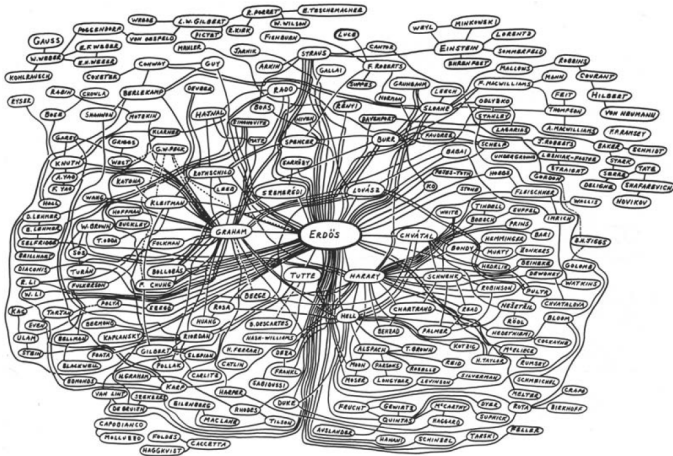
Estimator	$\hat{\Theta}^{VAR}$	$\hat{\Theta}^{missSBM}$	$\hat{\Theta}^{SVT}$	$\hat{\Theta}^{naive}$
$\ \mathbf{X} \odot (\mathbf{A} - \hat{\Theta})\ _2^2 / \ \mathbf{X} \odot \mathbf{A}\ _2^2$	0.312	0.317	0.357	0.541

Table: Normalized squared distance between the observed adjacency matrix for the network on interaction on Day 2, and its predicted value.

- ▶ The naive estimator $\hat{\Theta}^{naive}$:
 - ▶ $\hat{\Theta}_{ij}^{naive} = 1$ if an interaction between i and j has been recorded on Day 1
 - ▶ $\hat{\Theta}_{ij}^{naive} = 0$ if no such interaction has been recorded
 - ▶ $\hat{\Theta}_{ij}^{naive} = d/n$ if the information is missing, where d is the average degree of the graph for Day 1.

Conclusion

- ▶ **Least Squares Estimator:**
 - ▶ attains the optimal rates in a minimax sense
 - ▶ not realizable in polynomial time
- ▶ **(variational) MLE:**
 - ▶ minimax optimal
 - ▶ allows labels recovery
- ▶ Variational MLE has good performances in practice
- ▶ Can be used for **Link Prediction**



Thank You !