Asymptotic Relative Efficiency for Robust Estimation of the Mean of Contaminated Graphs under a Low Rank Model

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Problem

- **Given:** m networks on n vertices.
  - Each graph is represented as an adjacency matrix $A^{(t)} \in \mathbb{R}_{\geq 0}^{n \times n}$, $1 \leq t \leq m$.
  - Assuming that $A^{(t)}$ is symmetric and non-negative for $1 \leq t \leq m$.
  - We assume that the vertex correspondence is known.
- **Goal:** Estimate the mean of the collection of graphs.
  - Here mean of the graphs is defined as the average weight of an edge between each pair of vertices.
  - We are interested in the mean of the population of graphs.

Entrywise MLE $\hat{P}^{(1)}$

- Under the independent edge model (IEM), each edge A_{ij} independently follows some distribution (e.g. Bernoulli) with parameter P_{ij}.
- In this case, the entrywise MLE $\hat{P}^{(1)}$ is the entrywise mean $\bar{A}$.
  - Unbiased
  - UMVUE
- Problem solved!

Challenge

- What if we observe the graphs with contaminations?
- Even assuming that there is no contaminations, entrywise MLE $\hat{P}^{(1)}$ doesn't exploit any graph structure!
  - How can we take advantage of the unknown graph structure?

Stochastic Blockmodel

- One of the most important structures is the community structure in which vertices are clustered into different communities such that vertices of the same community behave similarly.
- The stochastic blockmodel (SBM) captures such structural property and is widely used in modeling networks.

Stochastic Blockmodel

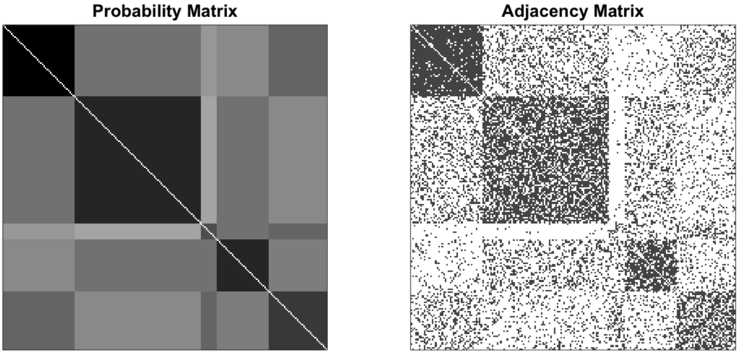


Figure: Example illustrating the SBM. The figure on the left is the probability matrix P that follows a SBM with $K = 5$ blocks; The other figure shows the adjacency matrix A for 200 vertices generated from the SBM with probability matrix P.

Stochastic Blockmodel

- For simplicity, the concepts below are all for Bernoulli distribution.
- Each of n vertices is assigned to exactly one of K blocks.
- The probability of an edge between two vertices depends only on their respective block memberships, and the presence of edges are conditionally independent given block memberships.
- It is parameterized by the block probability matrix $B \in [0,1]^{K \times K}$, and the block proportions $\rho \in (0,1)^K$ with $\sum_{k=1}^{K} \rho_k = 1$.
- Let τ_i denote the block to which vertex i is assigned, then they are independent with $P(\tau_i = k) = \rho_k$.
- The probability of an edge between vertices i and j is B_{τ_i, τ_j}.

Random Dot Product Graph

- Random dot product graph (RDPG)
  - Each vertex is associated with a latent position.
  - The presence or absence of edges are independent Bernoulli random variables conditioning on these latent positions.
  - The probability of an edge between two vertices is given by the dot product of the corresponding latent positions.
- An RDPG can be parameterized as an SBM with K blocks if there are only K distinct latent positions.
- We are going to analyze SBM in the RDPG setting.
- It motivates the estimator $\widetilde{P}^{(1)}$ based on adjacency spectral embedding.

Uncontaminated Model

- Under the stochastic block model with parameters (B, ρ), we have $X_i \stackrel{iid}{\sim} \sum_{k=1}^{K} \rho_k \delta_{\nu_k}$, where $\nu = [\nu_1, \cdots, \nu_K]^T \in \mathbb{R}^{K \times d}$ satisfies $B = \nu^T \nu$. Define the block assignment τ such that $\tau_i = k$ if and only if $X_i = \nu_k$. Let $P = XX^T$ where $X = [X_1, \cdots, X_n]^T$.
- First sample τ from the multinomial distribution with parameter ρ. Then we are going to sample m conditionally i.i.d. symmetric graphs $G^{(1)}, \cdots, G^{(m)}$ such that conditioning on τ, $G_{ij}^{(k)} \stackrel{ind}{\sim} \mathrm{Exp}(P_{ij})$ for each $1 \leq k \leq m$, $1 \leq i \leq j \leq n$.

Adjacency Spectral Embedding

- For an RDPG, the probability matrix $P = XX^T$ is symmetric, positive semidefinite and has rank at most d if $X \in \mathbb{R}^{n \times d}$.
- Let $A = [U_A|\widetilde{U}_A][S_A \oplus \widetilde{S}_A][U_A|\widetilde{U}_A]^T$ be the eigen-decomposition of A, where $S_A \in \mathbb{R}^{d \times d}$ is diagonal matrix with the d largest eigenvalues of A, and $U_A \in \mathbb{R}^{n \times d}$ is the matrix with orthonormal columns of the corresponding eigenvectors. Then the **adjacency spectral embedding (ASE)** of A to dimension d is given by $\widehat{X} = U_A S_A^{1/2}$.

Estimator $\widetilde{P}^{(1)}$

- Obtain $\hat{X}$ by applying ASE to entrywise mean $\hat{P}^{(1)}$ with dimension d.
- Define $\widetilde{P}^{(1)} = \hat{X}\hat{X}^T$ as an estimator of P.

Comparison between $\hat{P}^{(1)}$ and $\widetilde{P}^{(1)}$

To compare the performance between $\hat{P}^{(1)}$ and $\widetilde{P}^{(1)}$, since both of them are asymptotic unbiased, we examine the asymptotic relative efficiency (ARE), defined as: $\mathrm{ARE}(\hat{P}_{ij}^{(1)}, \widetilde{P}_{ij}^{(1)}) = \lim_{n\to\infty} \frac{\mathrm{Var}(\widetilde{P}_{ij}^{(1)})}{\mathrm{Var}(\hat{P}_{ij}^{(1)})}$.

Theorem

Fix m, for any i and j, conditioning on $X_i = \nu_{\tau_i}$ and $X_j = \nu_{\tau_j}$, we have

$$\mathrm{ARE}(\hat{P}_{ij}^{(1)}, \widetilde{P}_{ij}^{(1)}) = 0.$$

And for n large enough, we have the approximation

$$\mathrm{RE}(\hat{P}_{ij}^{(1)}, \widetilde{P}_{ij}^{(1)}) \approx \frac{1/\rho_{\tau_i} + 1/\rho_{\tau_j}}{n}.$$

Contaminated Model

- Under the stochastic block model with parameters (B, ρ), we have $X_i \overset{iid}{\sim} \sum_{k=1}^{K} \rho_k \delta_{\nu_k}$, where $\nu = [\nu_1, \cdots, \nu_K]^T \in \mathbb{R}^{K \times d}$ satisfies $B = \nu^T \nu$. Define the block assignment τ such that $\tau_i = k$ if and only if $X_i = \nu_k$. Let $P = XX^T$ where $X = [X_1, \cdots, X_n]^T$.
- Now we assume the observed edges are contaminated with probability ϵ.
- First sample τ from the multinomial distribution with parameter ρ. Then we are going to sample m conditionally i.i.d. symmetric graphs $A^{(1)}, \cdots, A^{(m)}$ such that conditioning on τ, $A_{ij}^{(t)} \overset{ind}{\sim} (1-\epsilon)\mathrm{Exp}(P_{ij}) + \epsilon \mathrm{Exp}(C_{ij})$ for each $1 \le t \le m$, $1 \le i \le j \le n$, where the contamination is $C = YY^T$.

Comparison between $\hat{P}^{(1)}$ and $\widetilde{P}^{(1)}$

$$\hat{P}^{(1)}$$

For any fixed m, or
$m = O(n^b)$ for $b > 0$,
any $1 \leq i, j \leq n$,
$\lim_{n\to\infty} \mathrm{Bias}^2(\hat{P}_{ij}^{(1)}) =$
$\lim_{n\to\infty} \mathrm{Bias}^2(\widetilde{P}_{ij}^{(1)})$
$\mathrm{Var}(\widetilde{P}_{ij}^{(1)})/\mathrm{Var}(\hat{P}_{ij}^{(1)})$
$= O(n^{-2}(\log n)^6)$

$$\widetilde{P}^{(1)}$$

Maximum L-q Likelihood Estimator

- With contaminations, the performance of MLE degrades.
- We should use entrywise robust estimator instead of $\hat{P}^{(1)}$.
- Maximum L-q Likelihood Estimator (MLqE) is an M-estimator with robust property.
- Denote MLqE as $\hat{P}^{(q)}$.
- MLE is a special case of MLqE with $q = 1$.

Comparison between $\hat{P}^{(1)}$ and $\hat{P}^{(q)}$

$\hat{P}^{(1)}$ $\longleftrightarrow$ $\hat{P}^{(q)}$

For any fixed n, C large enough, any $1 \le i, j \le n$,

$$\lim_{m\to\infty} \mathrm{Bias}^2(\hat{P}_{ij}^{(1)}) > \lim_{m\to\infty} \mathrm{Bias}^2(\hat{P}_{ij}^{(q)})$$

$$\lim_{m\to\infty} \mathrm{Var}(\hat{P}_{ij}^{(1)}) = \lim_{m\to\infty} \mathrm{Var}(\hat{P}_{ij}^{(q)}) = 0$$

$\hat{P}^{(1)}$ $\updownarrow$ $\widetilde{P}^{(1)}$

For any fixed m, or $m = O(n^b)$ for $b > 0$, any $1 \le i, j \le n$,

$$\lim_{n\to\infty} \mathrm{Bias}^2(\hat{P}_{ij}^{(1)}) = \lim_{n\to\infty} \mathrm{Bias}^2(\widetilde{P}_{ij}^{(1)})$$

$$\mathrm{Var}(\widetilde{P}_{ij}^{(1)})/\mathrm{Var}(\hat{P}_{ij}^{(1)}) = O(n^{-2}(\log n)^6)$$

Estimator $\widetilde{P}^{(q)}$

- $\hat{P}^{(q)}$ has the robust property while $\widetilde{P}^{(1)}$ has low asymptotic variance.
- Can we have both simultaneously?
- Define $\widetilde{P}^{(q)}$ as applying ASE to $\hat{P}^{(q)}$!

Comparison between $\widetilde{P}^{(q)}$ and $\hat{P}^{(q)}$

$$\begin{tikzcd}[column sep=huge, row sep=huge]
\hat{P}^{(1)} \arrow[rrr, leftrightarrow] \arrow[d, leftrightarrow] & & & \hat{P}^{(q)} \arrow[d, leftrightarrow] \\
\widetilde{P}^{(1)} & & & \widetilde{P}^{(q)}
\end{tikzcd}$$

Top arrow ($\hat{P}^{(1)} \leftrightarrow \hat{P}^{(q)}$):

For any fixed n, C large enough, any $1 \leq i,j \leq n$,
$\lim_{m\to\infty} \mathrm{Bias}^2(\hat{P}_{ij}^{(1)}) > \lim_{m\to\infty} \mathrm{Bias}^2(\hat{P}_{ij}^{(q)})$

$\lim_{m\to\infty} \mathrm{Var}(\hat{P}_{ij}^{(1)}) = \lim_{m\to\infty} \mathrm{Var}(\hat{P}_{ij}^{(q)}) = 0$

Left arrow ($\hat{P}^{(1)} \leftrightarrow \widetilde{P}^{(1)}$):

For any fixed m, or
$m = O(n^b)$ for $b > 0$,
any $1 \leq i,j \leq n$,
$\lim_{n\to\infty} \mathrm{Bias}^2(\hat{P}_{ij}^{(1)}) = \lim_{n\to\infty} \mathrm{Bias}^2(\widetilde{P}_{ij}^{(1)})$
$\mathrm{Var}(\widetilde{P}_{ij}^{(1)})/\mathrm{Var}(\hat{P}_{ij}^{(1)}) = O(n^{-2}(\log n)^6)$

Right arrow ($\hat{P}^{(q)} \leftrightarrow \widetilde{P}^{(q)}$):

For any fixed m, or
$m = O(n^b)$ for $b > 0$,
any $1 \leq i,j \leq n$,
$\lim_{n\to\infty} \mathrm{Bias}^2(\hat{P}_{ij}^{(q)}) = \lim_{n\to\infty} \mathrm{Bias}^2(\widetilde{P}_{ij}^{(q)})$
$\mathrm{Var}(\widetilde{P}_{ij}^{(q)})/\mathrm{Var}(\hat{P}_{ij}^{(q)}) = O(mn^{-2}(\log n)^6)$

Summary

$$\begin{tikzcd} \hat{P}^{(1)} \arrow[rrr, leftrightarrow] \arrow[d, leftrightarrow] & & & \hat{P}^{(q)} \arrow[d, leftrightarrow] \\ \widetilde{P}^{(1)} \arrow[rrr, leftrightarrow] & & & \widetilde{P}^{(q)} \end{tikzcd}$$

For any fixed n, C large enough, any $1 \leq i, j \leq n$,

$$\lim_{m\to\infty} \mathrm{Bias}^2(\hat{P}^{(1)}_{ij}) > \lim_{m\to\infty} \mathrm{Bias}^2(\hat{P}^{(q)}_{ij})$$

$$\lim_{m\to\infty} \mathrm{Var}(\hat{P}^{(1)}_{ij}) = \lim_{m\to\infty} \mathrm{Var}(\hat{P}^{(q)}_{ij}) = 0$$

For any fixed m, or $m = O(n^b)$ for $b > 0$, any $1 \leq i, j \leq n$,

$$\lim_{n\to\infty} \mathrm{Bias}^2(\hat{P}^{(1)}_{ij}) = \lim_{n\to\infty} \mathrm{Bias}^2(\widetilde{P}^{(1)}_{ij})$$

$$\mathrm{Var}(\widetilde{P}^{(1)}_{ij})/\mathrm{Var}(\hat{P}^{(1)}_{ij}) = O(n^{-2}(\log n)^6)$$

For any fixed m, or $m = O(n^b)$ for $b > 0$, any $1 \leq i, j \leq n$,

$$\lim_{n\to\infty} \mathrm{Bias}^2(\hat{P}^{(q)}_{ij}) = \lim_{n\to\infty} \mathrm{Bias}^2(\widetilde{P}^{(q)}_{ij})$$

$$\mathrm{Var}(\widetilde{P}^{(q)}_{ij})/\mathrm{Var}(\hat{P}^{(q)}_{ij}) = O(mn^{-2}(\log n)^6)$$

For sufficiently large m, n and C, any $1 \leq i, j \leq n$,

$$\lim_{m\to\infty} \mathrm{Bias}^2(\widetilde{P}^{(1)}_{ij}) > \lim_{m\to\infty} \mathrm{Bias}^2(\widetilde{P}^{(q)}_{ij})$$

For any fixed m, or $m = o(n^2(\log n)^{-6})$, any $1 \leq i, j \leq n$,

$$\lim_{n\to\infty} \mathrm{Var}(\widetilde{P}^{(1)}_{ij}) = \lim_{n\to\infty} \mathrm{Var}(\widetilde{P}^{(q)}_{ij}) = 0$$

Simulation Settings

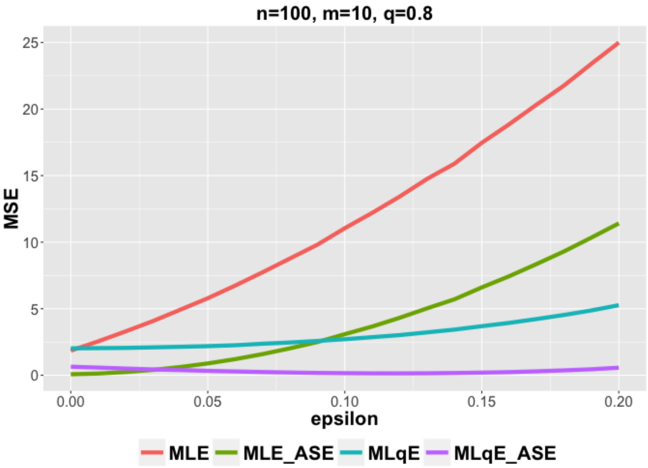
- Consider the stochastic blockmodel parameterized by

$$B = \begin{pmatrix} 4.2 & 2 \\ 2 & 7 \end{pmatrix} \text{ and } \rho = (0.5, 0.5).$$

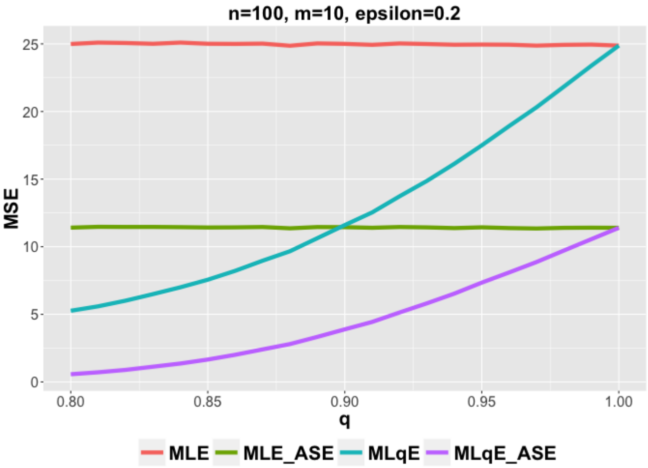
- The contamination is also a SBM parameterized by

$$C = \begin{pmatrix} 20 & 18 \\ 18 & 25 \end{pmatrix} \text{ and } \rho = (0.5, 0.5).$$

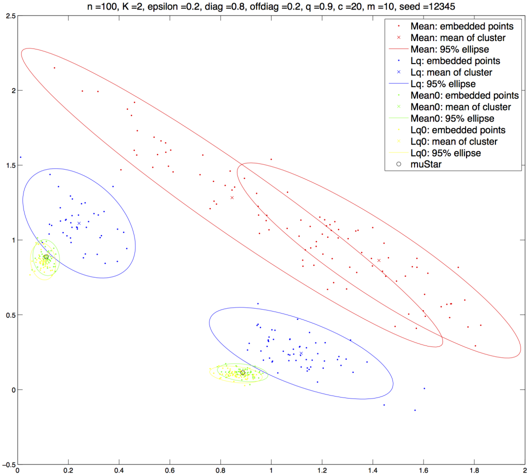
Simulation Results



Simulation Results



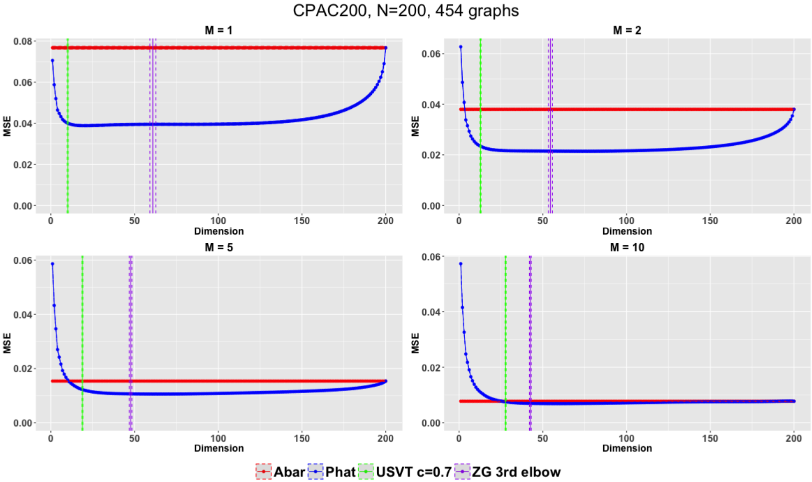
Scatter Plot of the Estimated Latent Positions $\widehat{X}_i$



CoRR Data Experiment

- 454 brain connectomes with 200 vertices generated from fMRI scans available at the Consortium for Reliability and Reproducibility (CoRR).
- Bootstrap resamples of size m from 454 graphs.

CoRR Data Experiment



Conclusion

- We propose an estimator for the mean of a collection of weighted graphs under a low rank random graph model.
- It not only inherits robustness from element-wise robust estimators but also has small variance due to application of a rank-reduction procedure.
- Under appropriate conditions, we prove that our estimator outperforms standard estimators via asymptotic relative efficiency.
- We illustrate our theory and methods by Monte Carlo simulation studies and experimental results, more is coming!

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