Model	and	Assumptions
0000	000	00

Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds

◆□▶ ◆□▶ ◆三▶ ◆三▶ ・三 ● のへで

Link prediction in graphs

Q. Duchemin

Université Paris Est Marne La Vallée

October 2020

Model and Assumptions	Penalised logistic loss	Performance of the penalised MLE	Computational lower bounds
00000000	000000	0000	000000

Goals of link prediction

- Understand, through a generative model, why different vertices are connected or not.
- Generalise these observations to the rest of the graph.

Motivations

- In social networks¹ Shared interests, differences in artistic tastes or political opinion.
- In biological networks² Interactions between molecules or protein.

^{1.} Wasserman, Faust et al., Social network analysis: Methods and applications.

^{2.} Madeira et Oliveira, "Biclustering algorithms for biological data analysis: a survey". 🚊 🗠 🧠 🤄

Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds

= 900

A large span of frameworks for link prediction

Supervised / Unsupervised?

Temporal aspect?

• Yes : Finding missing links.

• No :

- Links can be created and destroyed over time.
- $\bullet\,$ New nodes are entering the graph at each time step. 3

Topological-based link prediction ? Do we have additional features on the nodes $?^4$

Parametric or Non-parametric model?

Global or Local⁵ method?

Probabilistic / Geometric model?

^{3.} Dunlavy, Kolda et Acar, "Temporal link prediction using matrix and tensor factorizations".

^{4.} Wang, Satuluri et Parthasarathy, "Local probabilistic models for link prediction".

^{5.} Liben-Nowell et Kleinberg, "The link-prediction problem for social networks". $\epsilon \equiv F$

Model and AssumptionsPenalised logistic loss000000000000000

In this presentation, we will mainly be focused on

Baldin et Berthet, "Optimal link prediction with matrix logistic regression"

which proposed a method which is

- Not temporal
- Supervised
- Global method
- Probabilistic and Parametric

Motivation Adapt usual high-dimensional methods to a model with two covariates (explanatory variables).

Beyond link prediction, this paper allows to study

- Information-Computational gaps.
- General method to establish computational lower bounds.
- Classical statistical and optimization tools : Establishing minimax convergence rate and convex relaxation.

Model and Assumptions	Penalised logistic loss	Performance of the penalised MLE	Computational lower bounds
00000000	000000	0000	000000

▲□▶ ▲□▶ ▲三▶ ▲三▶ 三三 のへぐ

Model and Assumptions

2 Penalised logistic loss

Output Description of the penalised MLE



Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds

Section 1

Model and Assumptions

Model and Assumptions	Penalised logistic loss	Performance of the penalised MLE	Computational lower bounds
0000000	000000	0000	000000

We consider a graph G = ([n], E) with adjacency matrix $Y \in \{0, 1\}^{n \times n}$ generated from the following **generative model**.

- An explanatory variable $X_i \in \mathbb{R}^d$ is associated to each node $i \in [n]$.
- For some $\Theta_* \in \mathbb{S}^d$,

$$\forall i \in [n], \ Y_{i,i} = 0 \text{ and } \forall i, j \in [n]^2, \ i \neq j, \ Y_{i,j} \sim \mathcal{B}(\pi_{i,j}(\Theta_*)),$$

where

$$\pi_{i,j}: \mathbb{S}^d \to [0,1]$$
$$\Theta \mapsto \mathbb{P}\left((i,j) \in E\right) = \sigma(X_i^\top \Theta_* X_j) = \left(1 + \exp(-X_i^\top \Theta_* X_j)\right)^{-1}$$

・ロト ・ 母 ト ・ ヨ ト ・ ヨ ・ つへの

Observations

- For all $(i,j) \in \Omega$, $Y_{i,j}$ is observed.
- All the explanatory variables $(X_i)_i$ are known.

 Model and Assumptions
 Penalised logistic loss
 Performance of the penalised MLE
 Computational lower bounds

 00000000
 000000
 000000
 0000000

Comparaison with other models

Reformulation as a classical logistic regression problem using

$$X_i^{\mathsf{T}}\Theta_*X_j = \operatorname{Tr}(X_jX_i^{\mathsf{T}}\Theta_*) = \langle \operatorname{vec}(X_jX_i^{\mathsf{T}}), \operatorname{vec}(\Theta_*) \rangle.$$

- Generalised linear model.
- Graphon model with known explanatory variables.

• Trace regression models.

The model is $Y = \operatorname{Tr}(\Theta_*^{\mathsf{T}}Z) + \epsilon$ with $Z \in \mathbb{R}^{d_1 \times d_2}$ is a matrix of explanatory variables, $\Theta_* \in \mathbb{R}^{d_1 \times d_2}$ is the matrix of regression coefficients, $Y \in \mathbb{R}$ is the response and $\epsilon \in \mathbb{R}$ is the noise.

Metric learning.

Observations depend on an unknown geometric representation V_1, \ldots, V_n of the variables in a Euclidean space of low dimension. Based on noisy observations of $\langle V_i, V_j \rangle$, we want to recover $(V_i)_i$. Taking $X_i = e_i$ and $\Theta_* = V^\top V$ gives $\langle V_i, V_j \rangle = e_i^\top V^\top V e_j = X_i^\top \Theta_* X_j$.

Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds

Coping with the curse of dimensionality

High-dimensional setting $d^2 \gg N = |\Omega|$.

Motivation of the structural assumptions

$$\Theta_* = \sum_{l=1}^R \lambda_l u_l u_l^{\mathsf{T}}$$

The **affinity** $\Sigma_{i,j} \coloneqq X_i^\top \Theta_* X_j$ between vertices *i* and *j* is therefore only a function of the projections of X_i and X_j along the axes u_i i.e

$$\Sigma_{i,j} = \sum_{l=1}^{R} \lambda_l (u_l^{\mathsf{T}} X_i) (u_l^{\mathsf{T}} X_j).$$

Prior	Assumption
Only a few of the directions u_l have non- zero impact on the affinity	Θ_* is low-rank
Only few relevant coefficients of X_i and X_j influence the affinity	Sparsity on the u_l \Leftrightarrow Block-sparsity on Θ_*

Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds

▲ロ ▶ ▲周 ▶ ▲ 国 ▶ ▲ 国 ▶ ● の Q @

Block-sparse matrix logistic regression

<u>Notations</u> For any $p, q \in [0, \infty)$ and any $B \in \mathbb{S}^d$,

$$||B||_{p,q} = ||(||B_{1,*}||_p, \dots, ||B_{d,*}||_p)||_q,$$

where $B_{i,*}$ is the *i*-th row of *B*.

$$\forall B \in \mathbb{S}^n, \quad \|B\|_{F,\Omega}^2 \coloneqq \sum_{(i,j) \in \Omega} B_{i,j}^2.$$

For any $k, r \in [d]$ (with $r \leq k$),

$$\mathcal{P}_{k,r}(M) = \left\{ \Theta \in \mathbb{S}^d \ : \ \|\Theta\|_{1,1} < M, \ \|\Theta\|_{0,0} \le k, \ \text{and} \ \mathrm{rank}(\Theta) \le r \right\}$$

 $\|\cdot\|_{1,1}$ is the element wise l^1 norm on \mathbb{S}^d . $\|\cdot\|_{0,0}$ counts the number of selected variables.

Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds

▲ロ ▶ ▲周 ▶ ▲ 国 ▶ ▲ 国 ▶ ● の Q @

Recovering Θ_* from affinities

Block isometry property

For a matrix $\mathbb{X} \in \mathbb{R}^{d \times n}$ and an integer $s \in [d]$, we define $\Delta_{\Omega,s}(\mathbb{X}) \in (0,1)$ as the smallest positive real such that

$$N(1-\Delta_{\Omega,s}(\mathbb{X}))\|B\|_{F}^{2} \leq \|\mathbb{X}^{\top}B\mathbb{X}\|_{F,\Omega}^{2} \leq N(1+\Delta_{\Omega,s}(\mathbb{X}))\|B\|_{F}^{2},$$

for all matrices $B \in \mathbb{S}^d$ that satisfy the block-sparsity assumption $||B||_{0,0} \leq s$.

The Block isometry property guarantees that the matrix Θ_* can be recovered from observations of the affinities $\Sigma_{i,j}$.

Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds

・ロト ・ 母 ト ・ ヨ ト ・ ヨ ・ つへの

Block VS Restricted isometry property

Restricted isometry property

For a matrix $A \in \mathbb{R}^{n \times p}$ and an integer $s \in [p]$, $\delta_s(A) \in (0, 1)$ is the smallest positive real such that

$$n(1-\delta_s(A))\|v\|_2^2 \le \|Av\|_2^2 \le n(1+\delta_s(A))\|v\|_2^2,$$

for all *s*-sparse vectors, i.e. satisfying $||v||_0 \le s$. When $p = d^2$, we define $\delta_{\mathcal{B},s}(A)$ as the smallest positive real such that

$$n(1-\delta_{\mathcal{B},s}(A)) \|v\|_{2}^{2} \leq \|Av\|_{2}^{2} \leq n(1+\delta_{\mathcal{B},s}(A)) \|v\|_{2}^{2},$$

for all vectors such that v = vec(B), where B satisfies the block-sparsity assumption $||B||_{0,0} \le s$.

For a matrix $\mathbb{X} \in \mathbb{R}^{d \times n}$, let $\mathbb{D}_{\Omega} \in \mathbb{R}^{N \times d^2}$ be defined row-wise by $\mathbb{D}_{\Omega}(i,j) = \operatorname{vec}(X_j X_i^{\mathsf{T}})$ for all $(i,j) \in \Omega$. It holds that

 $\Delta_{\Omega,s}(\mathbb{X}) = \delta_{\mathcal{B},s}(\mathbb{D}_{\Omega}).$

Model and Assumptions Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds

▲ロ ▶ ▲周 ▶ ▲ 国 ▶ ▲ 国 ▶ ● の Q @

Recovering the affinities from the $\pi_{i,i}$

We do not directly observe the $\Sigma_{i,j}$, but their image through σ . A condition is necessary to ensure that the affinities can be recovered from the observed edges.

Identifiability Condition (IC)

There exists a constant M > 0 such that for all Θ in the class $\mathcal{P}_{d,d}(M)$ we have $\max_{(i,i)\in\Omega} |X_i^\top \Theta X_i| < M.$

Under (IC),

000000000

$$\forall (i,j) \in \Omega, \quad \inf_{\Theta \in \mathcal{P}_{d,d}(M)} \sigma'(X_i^{\mathsf{T}} \Theta X_j) \geq \mathcal{L}(M) > 0,$$

where $\mathcal{L}(M) \coloneqq \sigma'(M) = \sigma(M)(1 - \sigma(M))$.

Model and Assumptions	Penalised logistic loss	Performance of the penalised MLE	Computational lower bound
00000000	000000	0000	0000000
Preliminaries			

Log-likelihood

$$I_{Y}(\Theta) = -\sum_{(i,j)\in\Omega} \log\left(1 + e^{(2Y_{i,j}-1)X_{i}^{\top}\Theta X_{j}}\right)$$

 $-I_Y$ is a convex function of Θ .

Stochastic component of the likelihood

Denoting $I: \Theta \mapsto \mathbb{E}_{\Theta_*}[I_Y(\Theta)]$, it holds

$$I_{Y}(\Theta) - I(\Theta) = \sum_{(i,j)\in\Omega} (Y_{i,j} - \pi_{i,j}(\Theta_{*})) X_{i}^{\top} \Theta X_{j}$$
$$= \langle \langle \mathcal{E}_{\Omega}, \mathbb{X}^{\top} \Theta \mathbb{X} \rangle \rangle,$$

where $\mathcal{E}_{\Omega} = (Y_{i,j} - \pi_{i,j}(\Theta_*))_{(i,j)\in\Omega}$ with zeros on the complement Ω^c .

$$\begin{split} I(\Theta) - I(\Theta_*) &= -\sum_{(i,j)\in\Omega} \mathrm{KL}\left(\pi_{i,j}(\Theta_*), \pi_{i,j}(\Theta)\right) \\ &= -\mathrm{KL}\left(\mathbb{P}_{\Theta_*}, \mathbb{P}_{\Theta}\right). \end{split}$$

◆□▶ ◆□▶ ◆三▶ ◆三▶ 三三 - のへ⊙

Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds

Section 2

Penalised logistic loss

Model and Assumptions Penalised logistic loss Penalised logistic loss Penalised MLE Computational lower bounds Penalised logistic loss

$$\hat{\Theta} \in \underset{\Theta \in \mathcal{P}_{d,d}(M)}{\operatorname{arg\,min}} \left\{ -I_{Y}(\Theta) + p(\Theta) \right\}$$

with a penalty p defined by

$$p(\Theta) = g\left(\mathrm{rank}(\Theta), \|\Theta\|_{0,0}\right) \text{ with } g(R, K) = cKR + cK\log\left(\frac{de}{K}\right),$$

where c > 0 is a universal constant and to be specified further.

Non-asymptotic upper bound

Assume the design matrix X satisfies $\max_{(i,j)\in\Omega} |X_i^{\top}\Theta_*X_j| < M$ for some M > 0and all Θ_* in a given class. Then

$$\sup_{\Theta_* \in \mathcal{P}_{k,r}(M)} \frac{1}{N} \mathbb{E} \left[\mathrm{KL}(\mathbb{P}_{\Theta_*}, \mathbb{P}_{\hat{\Theta}}) \right] \leq C_1 \left\{ \frac{kr}{N} + \frac{k}{N} \log(\frac{de}{k}) \right\},$$

where $C_1 > 3c$ is some universal constant for all k = 1, ..., d and r = 1, ..., k.

Model and Assumptions	Penalised logistic loss	Performance of the penalised MLE	Computational lower
00000000	00000	0000	0000000
Proof (1/2)			

bounds

Let us recall that $I(\Theta) = \mathbb{E}_{\Theta_x} [I_Y(\Theta)]$ and that

$$I(\Theta_*) - I(\Theta) = \sum_{(i,j)\in\Omega} \operatorname{KL}\left(\pi_{i,j}(\Theta_*), \pi_{i,j}(\Theta)\right).$$

It suffices to show

$$\sup_{\Theta_{*}\in\mathcal{P}_{k,r}(M)}\mathbb{P}_{\Theta_{*}}\left(\underbrace{l(\Theta_{*})-l(\hat{\Theta})+p(\hat{\Theta})}_{:=\tau^{2}(\hat{\Theta},\Theta_{*})}>2p(\Theta_{*})+R_{t}^{2}\right)\leq e^{-cR_{t}}, \ (*)$$

for any $R_t > 0$ and some numeric constant c > 0. Indeed, then taking $R_t^2 = p(\Theta_*)$, it follows that $I(\Theta_*) - I(\hat{\Theta}) \leq 3p(\Theta_*)$ uniformly for all Θ_* in the considered class with probability at least $1 - e^{-c\sqrt{p(\Theta_*)}}$.

- On $\{\tau^2(\hat{\Theta}, \Theta_*) \leq 2p(\Theta_*)\}$, (*) clearly holds.
- On $\{\tau^2(\hat{\Theta},\Theta_*)>2p(\Theta_*)\}$

 $\langle\!\langle \mathcal{E}_{\Omega}, \mathbb{X}^{\mathsf{T}}(\hat{\Theta} - \Theta_{*})\mathbb{X}\rangle\!\rangle \geq l(\Theta_{*}) - l(\hat{\Theta}) + p(\hat{\Theta}) - p(\Theta_{*}) \geq \frac{1}{2}\tau^{2}(\hat{\Theta}, \Theta_{*}).$ ・ロト・西ト・ヨト・ヨト・ 日・

Model and Assumptions	Penalised logistic loss	Performance of the penalised MLE	Computational lower bounds
00000000	000000	0000	0000000
Proof (2/2)			

Therefore, for any $\Theta_* \in \mathcal{P}_{k,r}(M)$, we have

$$\mathbb{P}_{\Theta_*}(\tau^2(\hat{\Theta},\Theta_*) > 2p(\Theta_*) + R_t^2) \le \mathbb{P}_{\Theta_*}\left(\sup_{\tau(\Theta,\Theta_*) \ge R_t} \frac{\langle\!\langle \mathcal{E}_{\Omega}, \mathbb{X}^\top(\Theta - \Theta_*) \mathbb{X} \rangle\!\rangle}{\tau^2(\Theta,\Theta_*)} \ge \frac{1}{2}\right).$$

We apply the **peeling device** : we slice the set $\tau(\Theta, \Theta_*) \ge R_t$ into pieces on which the penalty term $p(\Theta)$ is fixed and the term $I(\Theta_*) - I(\Theta)$ is bounded.

$$\begin{split} & \mathbb{P}_{\Theta_{*}}\left(\sup_{\tau(\Theta,\Theta_{*})\geq R_{t}}\frac{\langle\!\langle \mathcal{E}_{\Omega}, \mathbb{X}^{\top}(\Theta-\Theta_{*})\mathbb{X}\rangle\!\rangle}{\tau^{2}(\Theta,\Theta_{*})}\geq\frac{1}{2}\right) \\ & \leq \sum_{K=1}^{d}\sum_{R=1}^{K}\sum_{s=1}^{\infty}\mathbb{P}_{\Theta_{*}}\left(\sup_{\substack{\Theta:R_{t}\leq\tau(\Theta,\Theta_{*})\leq 2^{s}R_{t}\\ \|\Theta\|_{0,0}=k, \mathrm{rank}(\Theta)=R}}\langle\!\langle \mathcal{E}_{\Omega}, \mathbb{X}^{\top}(\Theta-\Theta_{*})\mathbb{X}\rangle\!\rangle\geq\frac{1}{8}2^{2s}R_{t}^{2}\right). \end{split}$$

・ロト ・ 母 ト ・ ヨ ト ・ ヨ ・ つへの

To end the proof, we apply

- Bousquet's version of Talagrand's inequality.
- Dudley's entropy integral bound.

Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds

Going from KL to Σ and Θ .

Let us recall that $I(\Theta) = \mathbb{E}_{\Theta_*} \left[I_Y(\Theta) \right]$ and that

$$I(\Theta_*) - I(\Theta) = \sum_{(i,j)\in\Omega} \operatorname{KL}(\pi_{i,j}(\Theta_*), \pi_{i,j}(\Theta)).$$

Going from KL to Σ .

Using $\nabla I(\Theta_*) = 0$, it holds using Taylor expansion,

$$\begin{split} I(\Theta_{*}) - I(\hat{\Theta}) &= \frac{1}{2} \sum_{(i,j)\in\Omega} \sigma' \left(X_{i}^{\top} \Theta_{0} X_{j} \right) \langle\!\langle X_{j} X_{i}^{\top}, \Theta_{*} - \hat{\Theta} \rangle\!\rangle^{2} \\ &\geq \frac{\mathcal{L}}{2} \sum_{(i,j)\in\Omega} \langle\!\langle X_{j} X_{i}^{\top}, \Theta_{*} - \hat{\Theta} \rangle\!\rangle^{2} \\ &= \frac{\mathcal{L}}{2} \| \mathbb{X}^{\top} \left(\Theta_{*} - \hat{\Theta} \right) \mathbb{X} \|_{F,\Omega}^{2}, \end{split}$$

where $\Theta_0 \in [\hat{\Theta}, \Theta_*]$ element-wise.

Going from KL to Θ .

$$\frac{\mathcal{L}}{2}N\left(1-\Delta_{\Omega,d}\right)\|\Theta_*-\hat{\Theta}\|_F^2 \leq \frac{\mathcal{L}}{2}\|\mathbf{X}^\top\left(\Theta_*-\hat{\Theta}\right)\mathbf{X}\|_{F,\Omega}^2 \leq I(\Theta_*)-I(\hat{\Theta}).$$

Model and Assumptions	Penalised logistic loss	Performance of the penalised MLE	Computational lower bounds
Dradiction	00000	0000	000000
Prediction			

Measure the prediction error of an estimator $\hat{\Theta}$ by

$$\mathbb{E}\left[\sum_{(i,j)\in\Omega} \left(\pi_{i,j}(\hat{\Theta}) - \pi_{i,j}(\Theta_*)\right)^2\right],\$$

which is controlled according to the following result using the smoothness of the logistic function σ .

Solving link prediction Under (IC), $\sup_{\Theta_{\star} \in \mathcal{P}_{k,r}(M)} \frac{1}{2N} \mathbb{E} \left[\| \Sigma_{\star} - \hat{\Sigma} \|_{F,\Omega} \right] \leq \frac{C_1}{\mathcal{L}(M)} \left(\frac{kr}{N} + \frac{k}{N} \log(\frac{de}{k}) \right),$ with $C_1 > 0$.

・ロト ・ 母 ト ・ ヨ ト ・ ヨ ・ つへの

Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds

Section 3

Performance of the penalised MLE

Model and Assumptions Penalised logistic loss OCODOOO Performance of the penalised MLE Computational lower bounds OCODOOO CODOOO CODOO CODOO

The rank-constrained maximum likelihood estimators with bounded block size is

$$\hat{\Theta}_{k,r} \in \underset{\Theta \in \mathcal{P}_{k,r}}{\arg\min} \left\{ -I_{Y}(\Theta) \right\}.$$

Non-asymptotic upper bound on the rate of estimation

Assume the design matrix \mathbb{X} satisfies the block isometry property and $\max_{(i,j)\in\Omega} |X_i^{\top} \Theta_* X_j| < M$ for some M > 0 and all Θ_* in a given class. Then for the maximum likelihood estimator $\hat{\Theta}_{k,r}$,

$$\sup_{\Theta_* \in \mathcal{P}_{k,r}(M)} \mathbb{E}\left[\| \hat{\Theta}_{k,r} - \Theta_* \|_F^2 \right] \leq \frac{C_2}{\mathcal{L}(M)(1 - \Delta_{\Omega,2k}(\mathbb{X}))} \left\{ \frac{kr}{N} + \frac{k}{N} \log(\frac{de}{k}) \right\},$$

for all k = 1, ..., d and r = 1, ..., k and some constant $C_2 > 0$.

Model and Assumptions	Penalised logistic loss	Performance of the penalised MLE	Computational lower bounds
00000000	000000	0000	0000000
Lower bounds			

Minimax lower bound

Let the design matrix \mathbb{X} satisfy the block isometry property. Then for estimating $\Theta_* \in \mathcal{P}_{k,r}(M)$ in the matrix logistic regression model, the following lower bound on the rate of estimation holds

$$\inf_{\hat{\Theta}} \sup_{\Theta_{\star} \in \mathcal{P}_{k,r}(M)} \mathbb{E}\left[\| \hat{\Theta} - \Theta_{\star} \|_{F}^{2} \right] \geq \frac{C_{3}}{\left(1 + \Delta_{\Omega,2k}(\mathbb{X})\right)} \left(\frac{kr}{N} + \frac{k}{N} \log(\frac{de}{k}) \right),$$

where the constant $C_3 > 0$ is independent of d, k, r and the infimum extends overall estimators $\hat{\Theta}$.

The penalised maximum likelihood approach attains the minimax rate of estimation over simultaneously block-sparse and low-rank matrices.

Model and Assumptions F 000000000 000

Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds

Sparse matrix logistic regression

For any $k, r \in [d]$,

$$\hat{\Theta}_{Lasso} \in \underset{\Theta \in \mathbb{S}^d}{\arg\min} \{ -I_Y(\Theta) + \lambda \|\Theta\|_{1,1} \},\$$

with $\lambda > 0$ to be chosen further, which is equivalent to the logistic Lasso on $vec(\Theta)$.

Theorem

Assume the design matrix \mathbb{X} satisfies the block isometry property and $\max_{(i,j)\in\Omega} |X_i^{\mathsf{T}} \Theta X_j| < M$ for some M > 0 and all Θ_* in a given class. Then for $\lambda = C_4 \sqrt{\log d}$, where $C_4 > 0$ is an appropriate universal constant,

$$\sup_{\Theta_* \in \mathcal{P}_{k,r}(M)} \mathbb{E}\left[\| \hat{\Theta}_{Lasso} - \Theta_* \|_F^2 \right] \le \frac{C_5}{\mathcal{L}(M)(1 - \Delta_{\Omega,2k}(\mathbb{X}))} \frac{k^2}{N} \log d,$$

for all k = 1, ..., d and r = 1, ..., k and some universal constant $C_5 > 0$.

Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds

◆□▶ ◆□▶ ◆ □▶ ◆ □ ▶ ● □ ● ● ● ●

Section 4

Computational lower bounds

Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds 000000

The Planted Clique problem

Computational lower bound It is the fastest rate of estimation attained by a (randomised) polynomial-time algorithm in the worst-case scenario.

Idea : Detecting a subspace of $\mathcal{P}_{k,r}$ can be computationally as hard as solving the dense subgraph detection problem.

The Planted Clique problem

- G(n, 1/2) is the distribution of Erdos Renyi graphs
- G(n, 1/2, k, q) is the distribution of graphs constructed by
 - first picking k vertices independently at random.
 - connecting all edges in-between with probability $q \in (1/2, 1]$.
 - then joining each remaining pair of distinct vertices by an edge independently at random with probability 1/2.

Planted clique problem refers to the hypothesis testing problem of

 $\mathbb{H}_{0}: A \sim G(n, 1/2) \quad \mathbb{H}_{1}: A \sim G(n, 1/2, k, 1).$

based on observing a random graph A drawn from either G(n, 1/2) or G(n, 1/2, k, 1).

Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds

Dense subgraph detection

Planted Clique problemUnsolvablePlanted CliquePolynomial time $unsolvableConjecturealgorithm<math>2 \log_2 n$ $c \sqrt{n}$

Extension to the dense subgraph detection problem

$$\mathbb{H}_0: A \sim G(n, 1/2) \text{ vs } \mathbb{H}_1: A \sim G(n, 1/2, k, q), \quad q \in (1/2, 1]$$

The dense subgraph detection conjecture (DSD Conjecture)

For any sequence $k = k_n$ such that $k \le n^{\beta}$ for some $0 < \beta < 1/2$, and any $q \in (1/2, 1]$, there is no (randomised) polynomial-time algorithm that can correctly identify the dense subgraph with probability tending to 1 as $n \to \infty$, i.e. for any sequence of (randomised) polynomial-time tests $(\psi_n : \mathbb{G}_n \to \{0, 1\})_n$, we have

$$\liminf_{n\to\infty} \{\mathbb{P}_0(\psi_n(A) = 1) + \mathbb{P}_1(\psi_n(A) = 0)\} \ge 1/3.$$

Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds

Reduction to the dense subgraph detection problem

Sampling from $G(n, 1/2) \Leftrightarrow \Theta_0 = 0 \in \mathbb{R}^{d \times d}$ Sampling from G(n, 1/2, k, q)?

We consider

$$\begin{array}{l} \mathcal{N} = |\Omega| = {n \choose 2}, \\ \forall i \in [n], \ X_i = \mathcal{N}^{1/4} e_i \in \mathbb{R}^d. \\ \alpha_N = \frac{\alpha}{\sqrt{N}} \text{ for some } \alpha > 0. \end{array}$$



$$\mathcal{G}_{k}^{\alpha_{N}} \coloneqq \left\{ \Theta \in \mathcal{P}_{k,1}(M) \ : \ \exists S \in \mathcal{S}_{k}([n]) \text{ s.t. } \Theta_{i,j} = \left\{ \begin{array}{cc} \alpha_{N} & \text{if } i, j \in S \\ 0 & \text{otherwise.} \end{array} \right\}$$

Then for any $\Theta \in \mathcal{G}_k^{\alpha_N}$,

$$\mathbb{P}\left((i,j)\in E|X_i,X_j\right) = \left(1+e^{-X_i^{\top}\Theta X_j}\right)^{-1} = \begin{cases} (1+e^{-\alpha})^{-1} & \text{if } \Theta_{i,j} = \alpha_N\\ 1/2 & \text{otherwise.} \end{cases}$$

◆□> ◆□> ◆三> ◆三> ● □ ● ● ●

.

The testing problem

$$\mathbb{H}_0: Y \sim \mathbb{P}_{\Theta_0}$$
 vs $\mathbb{H}_1: Y \sim \mathbb{P}_{\Theta}, \Theta \in \mathcal{G}_k^{\alpha_N}.$

The dense subgraph detection problem with $q = (1 + e^{-\alpha})^{-1}$.

Computational lower bound of order k^2/N

Let \mathcal{F}_k be any class of matrices containing $\mathcal{G}_k^{\alpha_N} \cup \{\Theta_0\}$. Let c > 0 and f(k, d, N) with $f(k, d, N) \leq ck^2/N$ for $k = k_n < n^\beta, 0 < \beta < 1/2$ and a sequence $d = d_n$, for all $n > m_0 \in \mathbb{N}$.

If (DSD Conjecture) holds, for some design X that fulfils the block isometry property, for any estimator $\hat{\Theta}$, computable in polynomial time, there exists a sequence $(k, d, N) = (k_n, d_n, N)$, such that

$$\frac{1}{f(k,d,N)}\sup_{\Theta_*\in\mathcal{F}_k}\mathbb{E}\left[\|\hat{\Theta}-\Theta_*\|_F^2\right]\to+\infty.$$

・ロト ・ 母 ト ・ ヨ ト ・ ヨ ・ つへの

Let's sketch the proof!

 Model and Assumptions
 Penalised logistic loss

 000000000
 000000

Performance of the penalised MLE

Computational lower bounds

・ロト ・ 母 ト ・ ヨ ト ・ ヨ ・ つへの

Proof of the computational lower bound (1/2)

We here provide a proof of the computational lower bound on the prediction error. Assume that there exists a hypothetical estimator $\hat{\Theta}$ computable in polynomial time such that

$$\limsup_{n\to\infty}\frac{1}{f(k,d,N)}\sup_{\Theta_*\in\mathcal{F}_k}\frac{1}{N}\mathbb{E}\left[\|\mathbb{X}^{\mathsf{T}}(\hat{\Theta}-\Theta_*)\mathbb{X}\|_{F,\Omega}^2\right]\leq b<\infty,$$

for all sequences $(k, d, N) = (k_n, d_n, N)$ and a constant *b*. Then by Markov's inequality, we have

$$\frac{1}{N} \| \mathbb{X}^{\mathsf{T}} (\hat{\Theta} - \Theta_*) \mathbb{X} \|_{F,W}^2 \le uf(k, d, N),$$

for some numeric constant u > 0 with probability 1 - b/u for all $\Theta_* \in \mathcal{F}_k$. Following the reduction scheme, we consider the design vectors $X_i = N^{1/4}e_i$, i = 1, ..., n and the subset of edges Ω , such that

$$\frac{1}{N} \| \mathbb{X}^{\mathsf{T}} (\hat{\Theta} - \Theta_*) \mathbb{X} \|_{F,\Omega}^2 = \sum_{(i,j)\in\Omega} (\hat{\Theta}_{i,j} - (\Theta_*)_{i,j})^2 = \| \hat{\Theta} - \Theta_* \|_{F,\Omega}^2,$$

for any $\Theta_* \in \mathcal{G}_{\alpha_N k}$.

Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds

Proof of the computational lower bound (2/2)

Thus, in order to separate the hypotheses

$$\mathbb{H}_{0}: Y \sim \mathbb{P}_{0} \text{ vs. } \mathbb{H}_{1}: Y \sim \mathbb{P}_{\Theta}, \ \Theta \in \mathcal{G}_{k}^{\alpha_{N}},$$

it is natural to employ the following test

$$\psi(\mathbf{Y}) = \mathbb{1}\left\{\|\hat{\boldsymbol{\Theta}}\|_{F,\Omega} \geq \tau_{d,k}(u)\right\},\$$

where $\tau_{d,k}^2(u) = uf(k, d, N)$. The type *I* error of this test is controlled automatically : $\mathbb{P}_0(\psi = 1) \le b/u$. For the type *II* error,

$$\sup_{\Theta \in \mathcal{G}_{k}^{\alpha_{N}}} \mathbb{P}_{\Theta}(\psi = 0) = \sup_{\Theta \in \mathcal{G}_{k}^{\alpha_{N}}} \mathbb{P}_{\Theta}(\|\hat{\Theta}\|_{F,\Omega} < \tau_{d,k}(u))$$
$$\leq \sup_{\Theta \in \mathcal{G}_{k}^{\alpha_{N}}} \mathbb{P}_{\Theta}(\|\hat{\Theta} - \Theta\|_{F,\Omega} > \|\Theta\|_{F,\Omega} - \tau_{d,k}(u))$$
$$\leq b/u,$$

provided $k^2 \alpha_N^2 \ge 4\tau_{d,k}^2(u) = 4uf(k, d, N)$ which holds if $\alpha^2 \ge 4uc$. Hence, $\lim_{n \to \infty} \sup_{\theta \in \mathcal{G}_k^{\alpha_N}} \mathbb{P}_{\Theta}(\psi(Y) = 0) \le 2b/u < 1/3.$

596

Model and Assumptions	Penalised logistic loss	Performance of the penalised MLE	Computational lower bounds
Summary			

Statistical and computational trade-off in high-dimensional estimation.



・ロト ・ 母 ト ・ ヨ ト ・ ヨ ・ つへの

The computational gap is most noticeable for the matrices of rank 1.

Model and Assumptions	Penalised logistic loss	Performance of the penalised MLE	Computational lower bounds
Conclusion			

- The matrix logistic regression model is very natural to study the connection between **statistical accuracy** and **computational efficiency**.
- Block-sparsity is a **limiting model selection criterion** for polynomial-time estimation in the logistic regression model.
- With a larger parameter space, while the statistical rates might be worse, they might be closer to those that are computationally achievable.

• The logistic regression is also a representative of a large class of generalised linear models.

Model and Assumptions Penalised logistic loss Performance of the penalised MLE Computational lower bounds 000000 Performance of the penalised MLE Computational lower bounds 0000000 Performance of the second performance of the

Let $n, k \in \mathbb{N}^*$, $p = (p_1, \ldots, p_k)$ a probability vector and $W \in S_k([0, 1])$.

Definition : SBM

(X, G) is drawn under SBM(n, p, W) if :

•
$$X_u \sim p, \forall u \in [n].$$

•
$$G_{u,v} \sim \mathcal{B}(W(X_u, X_v)), v \in [n], u \neq v.$$

Definition : Agreement

Let $x, y \in [k]^n$.

$$A(x,y) = \max_{\pi \in S_k} \frac{1}{n} \sum_{u=1}^n \mathbb{1}_{x_u = \pi(y_u)}.$$

▲ロ ▶ ▲周 ▶ ▲ 国 ▶ ▲ 国 ▶ ● の Q @

Exact Recovery : $\mathbb{P}(A(X, \hat{X}) = 1) = 1 - o(1).$ \longrightarrow No IC gap.

Penalised logistic loss

Performance of the penalised MLE

Computational lower bounds

Information-Computational gap : the example of the SBM

Definition : Weak recovery

WR requires us to separate at least two communities. Weak recovery is solvable in SBM(n, p, W) if :

 $\exists \epsilon > 0, i, j \in [k]$, and an algo returning a partition (S, S^c) of [n] s.t.

$$\mathbb{P}\left(\frac{|\Omega_i \cap S|}{|\Omega_i|} - \frac{|\Omega_j \cap S|}{|\Omega_j|} \ge \epsilon\right) = 1 - o(1),$$

where $|\Omega_i| = \{ u \in [n] : X_u = i \}$.



 \rightarrow No IC gap for k = 2 and the conjecture from Decelle and al. states that there is an IT gap for $k \ge 3$.

▲□▶ ▲□▶ ▲□▶ ▲□▶ ▲□ ● ● ●