K-means: Relaxation and Correction

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Joint works with C. Giraud, F. Bunea and M. Royer.

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Clustering arises in various contexts



Clustering features



Clustering graphs



Topic of the talk

- K-means (relaxed or not) must and can be debiased
- we derive some non-asymptotic partial recovery bounds for a relaxed K-means
- some optimality in terms of exponential exponent

Main message

A corrected convex relaxation of K-means achieves some rate-optimal performances in various settings including (conditional) mixture of sub-Gaussian and (conditional) Stochastic Block Model.

Only tuning Parameter is K





3 Corrected K-means

- 4 Partial Recovery bounds ■ subGaussian Mixtures
 - Stochastic Block Models

Mixture of subGaussian variables Pearson('1895)

Partition

Partition
$$G^* = \{G_1^*, \dots, G_K^*\}$$
 of $\{1, \dots, n\}$

Mixture of subGaussian variables (conditional)

 $X_1,\ldots,X_n\in\mathbb{R}^p$ are independent with

• $\mathbb{E}[X_a] = \mu_k$ if $a \in G_k^*$

•
$$\Sigma_a^{-1/2} X_a$$
 is SubGauss $(L^2 I_p)$ where $\Sigma_a = \operatorname{Cov} (X_a)$ and $L \ge 1$.

The observations are gathered in $\mathbf{X} = [X_1, \dots, X_n] \in \mathbb{R}^{p imes n}$



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The observations are gathered in $\mathbf{X} = [X_1, \dots, X_n] \in \mathbb{R}^{p \times n}$



Objective : recovering G^* from **X** (μ and **\Sigma** are unknown but K is known)

Stochastic Block Model (SBM)

Holland et al(83), Abbe('17),

Let $\mathbf{X} = \operatorname{adjacency} \operatorname{matrix} \operatorname{of} \operatorname{an} \operatorname{undirected} \operatorname{graph} \in \{0, 1\}^{n \times n}$.

Let $\mathbf{Q} \in [0, 1]_{sym}^{K \times K}$

(conditional) SBM

The graph is generated by a SBM with partition G^* and matrix ${\bf Q}$ if ${\bf X}_{ab}$ with a < b are independent and

 $\mathbb{P}[\mathbf{X}_{ab} = 1] = \mathbf{Q}_{jk} \quad \text{for any } a \in G_j^* \text{ and } b \in G_k^* \ ,$

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Membership Matrix $\mathbf{A} \in \{0,1\}^{n \times K}$ defined by $\mathbf{A}_{ak} = \mathbf{1}_{a \in G_k}$ (or equivalently function $k : [n] \mapsto [K]$) is NOT Identifiable. Why?

Membership Matrix $\mathbf{A} \in \{0,1\}^{n \times K}$ defined by $\mathbf{A}_{ak} = \mathbf{1}_{a \in G_k}$ (or equivalently function $k : [n] \mapsto [K]$) is at best identifiable up to permutation

A more suitable object : The $n\times n$ Partnership matrix $\mathbf{B}^*=\mathbf{A}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T$

$$\mathbf{B}^*_{ab} = \begin{cases} \frac{1}{|G^*_k|} & \text{if } a \text{ and } b \text{ belong to the same } G^*_k \\ 0 & \text{else} \end{cases}$$

Invariant with respect to the group labeling.

 $\widehat{G} \in \arg\min_{G} \mathsf{Crit}(\mathbf{X}, G)$ where

$$\mathsf{Crit}(\mathbf{X}, G) = \sum_{k=1}^{K} \sum_{a \in G_k} \|X_a - \overline{X}_{G_k}\|^2 ,$$

where $\overline{X}_{G_k} = \frac{1}{|G_k|} \sum_{a \in G_k} X_a$

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- 2 Update the partition



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Two steps :

- Compute the centroids
- 2 Update the partition



Two caveats :

- There can be many local optima.
- In worst-case solving K-means is NP-hard (Mahajan et al.('09))

Rewriting K-means

$$\begin{aligned} \mathsf{Crit}(\mathbf{X},G) &= \sum_{k} |G_{k}| \|\overline{X}_{G_{k}}\|^{2} - 2 \sum_{a,b \in G_{k}} \langle X_{a}, X_{b} \rangle \frac{1}{|G_{k}|} + \sum_{a} \|X_{a}\|^{2} \\ &= -\sum_{k} \sum_{a,b \in G_{k}} \langle X_{a}, X_{b} \rangle \frac{1}{|G_{k}|} + \dots \\ &= -\langle \mathbf{X}^{T} \mathbf{X}, \mathbf{B} \rangle + \dots \end{aligned}$$

Rewriting *K*-means

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Lemma (Peng & Wei(07))

The K-means minimizer \widehat{G} satisfies

$$\begin{split} \widehat{\mathbf{B}} &\in \arg\min_{\mathbf{B}\in\mathcal{D}} \langle -\mathbf{X}^T\mathbf{X}, \mathbf{B} \rangle \ , \\ &\bullet \mathbf{B} \succcurlyeq 0 \\ &\bullet \sum_a \mathbf{B}_{ab} = 1, \forall b \\ \mathbf{B} &\in \mathbb{R}^{p \times p} : \bullet \mathbf{B}_{ab} \geqslant 0, \ \forall a, b \\ &\bullet \operatorname{Tr}(\mathbf{B}) = K \\ &\bullet \mathbf{B}^2 = \mathbf{B} \end{split}$$

Proof : Perron-Frobenius

Relaxed K-means

Idea : drop the $\mathbf{B}^2 = \mathbf{B}$ condition.

1 Estimate \mathbf{B}^* using the semi-definite program (SDP)

$$\widehat{\mathbf{B}} = \operatorname*{arg\,min}_{\mathbf{B} \in \mathcal{C}} \langle -\mathbf{X}^T \mathbf{X}, \mathbf{B} \rangle$$

where

$$\mathcal{C} := \begin{cases} \mathbf{o} \ \mathbf{B} \succeq 0 \\ \mathbf{b} \sum_{a} \mathbf{B}_{ab} = 1, \ \forall b \\ \mathbf{o} \ \mathbf{B}_{ab} \ge 0, \ \forall a, b \\ \mathbf{o} \ \mathrm{Tr}(\mathbf{B}) = K \end{cases}$$

2 (Compute \widehat{G} by applying any clustering algorithm on $\widehat{\mathbf{B}}$)

Remark :

- Convex optimization but many constraints : https://cims.nyu.edu/~villar/mnist.html
- No information of the group sizes are needed.

A second relaxation : Spectral Clustering

Spectral Clustering

- 1 Compute the matrix $\widehat{\mathbf{U}}$ made of the K-leading eigenvectors of $\mathbf{X}^T \mathbf{X}$
- **2** Estimate \widehat{G} by distance clustering on the rows of $\widehat{\mathbf{U}}$.

(e.g. Apply an approximate K-means algorithm to the rows of the matrix $\widehat{\mathbf{U}}$)

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Lemma (2019 & Wal(02)) Spectral Clustering is equivalent to 1 Estimate \mathbf{B}^* using the semi-definite program (SDP) $\overline{\mathbf{B}} = \arg\min_{\mathbf{B}\in\overline{\mathcal{C}}} \langle -\mathbf{X}^T\mathbf{X}, \mathbf{B} \rangle$ $\mathbf{B} \in \overline{\mathcal{C}}$ $\overline{\mathcal{C}} := \left\{ \mathbf{B} \in \mathbb{R}^{p \times p} : \begin{array}{c} \bullet \ 1 \succcurlyeq \mathbf{B} \succcurlyeq 0 \\ \bullet \ \mathrm{Tr}(\mathbf{B}) = K \end{array} \right\}$ 2 Compute \widehat{G} by distance clustering on the rows of $\overline{\mathbf{B}}$

 $\begin{array}{l} \Longrightarrow \text{ it amounts to dropping the constraints } \mathbf{B}1=1, \ \mathbf{B}_{ab} \geq 0 \text{ in the former relaxation} \\ \hline \frac{\operatorname{Proof}}{2} : 1) \ \mathbf{\overline{B}} = \widehat{\mathbf{U}} \widehat{\mathbf{U}}^T \\ 2) \ (\widehat{\mathbf{U}} \widehat{\mathbf{U}}^T)_{a \bullet} \text{ is some orthogonal transformation of } \widehat{\mathbf{U}}_{a \bullet}. \end{array}$





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Stochastic Block Models

Wikipedia knows

$$\mathsf{Crit}_K(G) = \sum_{k=1}^K \sum_{a \in G_k} \|X_a - \overline{X}_{G_k}\|^2$$



Quantization rather than clustering https://en.wikipedia.org/wiki/K-means_clustering

A simple model

Assume that the "points" X_a are independent random variables with

$$\mathbb{E}[X_a] = \mu_a$$
 and $\operatorname{Tr}(\operatorname{Cov}(X_a)) = \Gamma_a$.

$$\operatorname{Crit}_{K}(G) = \sum_{k=1}^{K} \sum_{a \in G_{k}} \|X_{a} - \overline{X}_{G_{k}}\|^{2}$$

Expected value at G

For a partition G we have

$$\mathbb{E}[\operatorname{Crit}_K(G)] = \frac{1}{2} \sum_k \frac{1}{|G_k|} \sum_{a, b \in G_k} \|\mu_a - \mu_b\|^2 + \sum_a \Gamma_a - \sum_k \frac{1}{|G_k|} \sum_{a \in G_k} \Gamma_a$$

 \longrightarrow tends to split "wide" clusters : a correction is needed !

Caveat (alternative view)

Recall our Minimization Problem : $\langle -\mathbf{X}^T\mathbf{X}, \mathbf{B} \rangle$

sGaussian Mixtures are of the form : $X_a = \mathbb{E}[X_a] + E_a = Information + Noise$,

$$\mathbb{E}[\mathbf{X}^T \mathbf{X}] = \mathbb{E}[\mathbf{X}]^T \mathbb{E}[\mathbf{X}] + \mathbf{\Gamma} , \qquad \text{where } \mathbf{\Gamma}_{aa} = \operatorname{Tr}[\operatorname{Cov}(E_a)]$$

Population K-means vs Ideal K-means

$$\begin{array}{lll} \mathbf{B}^{pop} & = & \arg\min_{\mathbf{B}\in\mathcal{D}} \langle -\,\mathbb{E}[\mathbf{X}]^T\,\mathbb{E}[\mathbf{X}] - \mathbf{\Gamma}, \mathbf{B} \rangle \\ \mathbf{B}^{id} & = & \arg\min_{\mathbf{B}\in\mathcal{D}} \langle -\,\mathbb{E}[\mathbf{X}]^T\,\mathbb{E}[\mathbf{X}], \mathbf{B} \rangle \end{array}$$

- Since $Tr[\mathbf{B}] = K$, we have $\mathbf{B}^{pop} = \mathbf{B}^{id}$ when $\Gamma = \gamma \mathbf{I}$.
- For heterogenerous Γ, B^{pop}_{aa} tends to take large values for large Γ_{aa} (it splits wide clusters).

Remark : If we knew the groups, we could estimate $\Gamma = \operatorname{diag}(\Gamma_1, \ldots, \Gamma_n)$ by

$$\widehat{\mathbf{\Gamma}}_{aa} = \langle X_a - X_{ne_1(a)}, X_a - X_{ne_2(a)} \rangle$$

with $ne_1(a)$ and $ne_2(a)$ two "neighbors" of a.

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Definition

Then, the estimator $\widehat{\Gamma}$ is the diagonal matrix defined by

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Definition

$$\begin{split} & \mathsf{Set}\; U(a,b) := \max_{c,d \in [n] \setminus \{a,b\}} \left| \left\langle X_a - X_b, \frac{X_c - X_d}{\|X_c - X_d\|} \right\rangle \right| \text{ and } \\ & \widehat{ne}_1(a) := \operatorname*{arg\,min}_{b \in [n] \setminus \{a\}} U(a,b) \; \text{ and } \; \widehat{ne}_2(a) := \operatorname*{arg\,min}_{b \in [n] \setminus \{a, \widehat{ne}_1(a)\}} U(a,b) \end{split}$$

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Corrected relaxed K-means (Bunea et al.('16))

Solve the SDP

$$\widehat{B} \in \underset{\mathbf{B} \in \mathcal{C}}{\operatorname{argmin}} \langle -\mathbf{X}^T \mathbf{X}, \mathbf{B} \rangle ,$$

with

$$\mathcal{C} := \begin{cases} \mathbf{B} \succeq \mathbf{0} \\ \mathbf{B} \in \mathbb{R}^{n \times n} : & \stackrel{\mathbf{O}}{\underset{ab}{\sum}} \stackrel{\mathbf{B} \succeq \mathbf{0}}{\underset{ab}{\sum}} \stackrel{\mathbf{I}, \forall b}{\underset{ab}{\sum}} \\ & \stackrel{\mathbf{B} = \mathbf{B}}{\underset{ab}{\sum}} \stackrel{\mathbf{I}, \forall b}{\underset{ab}{\sum}} \\ & \stackrel{\mathbf{I}, \forall b}{\underset{ab}{\sum}} \stackrel{\mathbf{I}, \forall b}{\underset{ab}{\sum} \\ & \stackrel{\mathbf{I}, \forall b}{\underset{ab}{\sum}} \\ & \stackrel{\mathbf{I}, \forall b}{\underset{ab}{\sum} \\ & \stackrel{\mathbf{I}, \forall b}{\underset{ab}{\sum}} \\ & \stackrel{\mathbf{I}, \forall b}{\underset{ab}{\sum} \\ & \stackrel{\mathbf{I}, \forall b}{\underset{ab}{\sum} \\ & \stackrel{\mathbf{I}, \forall b}{\underset{ab}{\sum} \\ & \stackrel{\mathbf{I}, \forall b}{\underset{ab}{\sum}} \\ & \stackrel$$

Similarly, one may define a corrected spectral clustering.

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$$\widehat{B} \in \underset{\mathbf{B} \in \mathcal{C}}{\operatorname{argmin}} \langle \widehat{\Gamma} - \mathbf{X}^T \mathbf{X}, \mathbf{B} \rangle ,$$

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Similarly, one may define a corrected spectral clustering.





3 Corrected K-means

4 Partial Recovery bounds ■ subGaussian Mixtures

Stochastic Block Models

Proportion of misclustered points

$$err(\widehat{G}, G^*) = \min_{\pi \in \mathcal{S}_K} \frac{1}{2n} \sum_{k=1}^K \left| G_k^* \triangle \widehat{G}_{\pi(k)} \right|$$

Our goal

Prove that with high-probability, when $s^2 \mbox{ is large }$

prop. misclustered =
$$err(\widehat{G}, G^*) \le e^{-cs^2}$$

where s^2 is an appropriate SNR.

Other related goals :

- **partial recovery** : Find the minimal s^2 such that $err(\hat{G}, G^*)$ is smaller than random guess whp.
- Perfect recovery : Find the minimal s^2 such that $err(\widehat{G}, G^*) = 0$ whp.

Mixture of subGaussian variables

 $X_1, \ldots, X_n \in \mathbb{R}^p$ are independent with

$$\mathbb{E}[X_a] = \mu_k \text{ if } a \in G_k^*$$
$$\mathbb{\Sigma}_a^{-1/2} X_a \text{ is SubGauss}(L^2 \mathbf{I}_p) \text{ where } \mathbb{\Sigma}_a = \operatorname{cov}(X_a)$$

We set

$$\Delta^2 = \min_{j \neq k} \|\mu_k - \mu_j\|^2, \quad \sigma^2 = L^2 \max_k |\boldsymbol{\Sigma}_k|_{op} \quad \text{and} \quad R_{\boldsymbol{\Sigma}} = \max_k \frac{|\boldsymbol{\Sigma}_k|_F^2}{|\boldsymbol{\Sigma}_k|_{op}^2},$$

and define the SNR

$$s^2 = \frac{\Delta^2}{\sigma^2} \wedge \frac{m\Delta^4}{R_{\Sigma}\sigma^4},$$

where \boldsymbol{m} denotes the size of the smallest cluster.

Toy Examples

Simplification : K = 2, $|G_1^*| = |G_{-1}^*| = n/2$, $\Sigma_1 = \Sigma_{-1} = \sigma^2 \mathbf{I}_p$, $\mu_{-1} = -\mu_1$.

Simplified Model $1: \mu_1$ is known. Bayes Classifier achieves :

$$\mathbb{E}[err(\widehat{G}, G^*)] = 2 \mathbb{P}[\mathcal{N}(0, \sigma^2) > \|\mu_1\|] \le 2 \exp\left[-\frac{\Delta^2}{8\sigma^2}\right]$$

Simplified Model 2 : μ_1 is sampled uniformly on the sphere of radius $\Delta/2$. Labels $Z_a \in \{-1, 1\}$ for $a = 1, \ldots, n$ are known.

Objective : classify a new observation X.

Optimal Classifier : $\hat{h}(x) = \operatorname{sign}\left(\left\langle \frac{1}{n} \sum_{a=1}^{n} Z_a X_a, x \right\rangle\right)$:

- $\blacksquare \text{ achieves the rate } e^{-c\Delta^2/\sigma^2} \text{ if } \tfrac{\Delta^2}{\sigma^2} \gtrsim 1 \vee \tfrac{p}{n}.$
- $\ \ \, \hbox{ achieves the rate } e^{-cn\Delta^4/(p\sigma^4)} \ \hbox{if } 1 \vee \sqrt{\frac{p}{n}} \lesssim \frac{\Delta^2}{\sigma^2} \lesssim 1 \vee \frac{p}{n}.$

See Ndaoud('18) for proper lower bounds.

$$s^2 = \frac{\Delta^2}{\sigma^2} \wedge \frac{m\Delta^4}{R_{\Sigma}\sigma^4},$$

Theorem (Giraud and V. ('18))

If $s^2 \gtrsim n/m$ (+ mild assumption), then $\mathbb{P}\left[err(\widehat{G}, G^*) > e^{-cs^2}\right] \lesssim \frac{1}{n^2}$.

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$$s^2 \gtrsim n/m$$
 is equivalent to $\Delta^2 \gtrsim \sigma^2 \frac{n}{m} \left(1 \lor \sqrt{\frac{R_{\Sigma}}{n}} \right) = \sigma^2 K \left(1 \lor \sqrt{\frac{R_{\Sigma}}{n}} \right).$

Remarks :

1 s^2 reduces to Δ^2/σ^2 when $\Delta^2/\sigma^2 \ge R_{\Sigma}/m$ Fei and Chen ('18), See Lu and Zhou ('16), Ndaoud('18) for sharp constants

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- $\begin{array}{ll} \mbox{2} & \mbox{perfect recovery for s^2}\gtrsim \log(n) \lor (n/m) & = \log(n) \lor K \\ \mbox{Dependency in K is suboptimal.} \\ & \mbox{Vempala and Wang('04) } \rightsquigarrow s^2 \gtrsim \log(n) \lor \sqrt{K \log(n)} \mbox{ when $n \gg p^3$.} \end{array}$

3 Do not cover the case where the proportion of error is $\geq e^{-c''K}$.

Benefit of Corrected K-means

Mild price for Γ estimation : $\frac{\|\mathbf{\Sigma}_k\|_{op} \operatorname{Tr}(\mathbf{\Sigma}_k)}{\|\mathbf{\Sigma}_k\|_F^2} \lesssim \frac{n}{\log(n)}$

$$\mathsf{Mild price for } \boldsymbol{\Gamma} \text{ estimation}: \frac{\|\boldsymbol{\Sigma}_k\|_{op} \mathrm{Tr}(\boldsymbol{\Sigma}_k)}{\|\boldsymbol{\Sigma}_k\|_F^2} \lesssim \frac{n}{\log(n)}$$

Without correction, additional assumption is required :

$$\Delta^2 \gtrsim \frac{\max \mathbf{\Gamma}_a - \min \mathbf{\Gamma}_a}{m}$$

For a balanced Partition, it amounts to

$$\Delta^2 \gtrsim \sigma^2 K \left(1 \vee \sqrt{\frac{R_{\boldsymbol{\Sigma}}}{n}} \vee \frac{\max_k tr[\boldsymbol{\Sigma}_k] - \min_k tr[\boldsymbol{\Sigma}_k]}{n} \right)$$

Simple Versions : All $\|\mu_i - \mu_j\|_2$ are equal

Step $1: |\widehat{\mathbf{B}} - \mathbf{B}^*|_1$ small implies that $err(\widehat{G}, G)$ is small.

New Objective : Show that $\langle \mathbf{X}^T \mathbf{X} - \widehat{\Gamma}, \mathbf{B}^* - \mathbf{B} \rangle > 0$ as long as $|\mathbf{B}^* - \mathbf{B}|_1$ is not small

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$$\begin{split} \langle \mathbf{X}^T \mathbf{X} - \widehat{\mathbf{\Gamma}}, \mathbf{B}^* - \mathbf{B} \rangle &= \langle \mathbf{A} \mu \mu^T \mathbf{A}^T, \mathbf{B}^* - \mathbf{B} \rangle + \langle \mathbf{E}^T \mathbf{E} - \mathbf{\Gamma}, \mathbf{B}^* - \mathbf{B} \rangle \\ &+ \langle \mathbf{\Gamma} - \widehat{\mathbf{\Gamma}}, \mathbf{B}^* - \mathbf{B} \rangle + \langle \mathbf{A} \mu \mathbf{E}^T + \mathbf{E} \mu \mathbf{A}^T, \mathbf{B}^* - \mathbf{B} \rangle \end{split}$$

We focus on the two first terms

Signal Term : $\langle \mathbf{A}\mu\mu^T \mathbf{A}^T, \mathbf{B}^* - \mathbf{B} \rangle = \frac{1}{4}\Delta^2 |\mathbf{B}^* - \mathbf{B}^* \mathbf{B}|_1$

Control of the quadratic term : $\langle {f E}^T {f E} - {f \Gamma}, {f B}^* - {f B} angle$

 \mathbf{B}^* is projection operator that averages over element of the same group. \rightsquigarrow Decomposition of $\mathbf{E}^T \mathbf{E} - \mathbf{\Gamma}$ by applying \mathbf{B}^* or $(\mathbf{I} - \mathbf{B}^*)$.

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Step 3 : Control of the Projection Along $\mathrm{Im}(\mathbf{B}^*)$

$$\begin{aligned} \langle (\mathbf{I} - \mathbf{B}^*)(\mathbf{E}^T \mathbf{E} - \mathbf{\Gamma})(\mathbf{I} - \mathbf{B}^*), \mathbf{B}^* - \mathbf{B} \rangle &\leq & \|\mathbf{E}^T \mathbf{E} - \mathbf{\Gamma}\|_{op} \|(\mathbf{I} - \mathbf{B}^*)[\mathbf{B}^* - \mathbf{B}](\mathbf{I} - \mathbf{B}^*)\|_* \\ &= \|\mathbf{E}^T \mathbf{E} - \mathbf{\Gamma}\|_{op} \frac{1}{2m} |\mathbf{B}^* - \mathbf{B}^* \mathbf{B}|_1 \end{aligned}$$

 \rightsquigarrow Concentration of $\mathbf{E}^T\mathbf{E}$ in operator norm

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Step 4 : Control of $\langle \mathbf{B}^* (\mathbf{E}^T \mathbf{E} - \mathbf{\Gamma}), \mathbf{B}^* - \mathbf{B} \rangle$.

A First try : $\langle \mathbf{A}, \mathbf{B} \rangle \leq |\mathbf{A}|_{\infty} |\mathbf{B}|_1$ does not lead to exponential bounds.

A Second try (Fei and Chen('17)) : $\langle \mathbf{A}, \mathbf{B} \rangle \leq \sum_{i=1}^{|\mathbf{B}|_1} \mathbf{A}_{(i)}$, where $\mathbf{A}_{(1)} \geq \mathbf{A}_{(2)} \geq \dots$ Control of the order statistics $\mathbf{B}^* (\mathbf{E}^T \mathbf{E} - \mathbf{\Gamma})$ by Hanson-Wright inequality + Union bound

(conditional) SBM

Assume that the graph is generated by a SBM with \mathbf{Q}_{jk} = probability of connection between nodes of groups j and k.

Let $\mathbf{X} = adjacency matrix of the graph \in \{0, 1\}^{n \times n}$.

For
$$a \in G_k^*$$
: $X_a = [\mathbf{QA}]_{k:} - \mathbf{Q}_{kk}e_a + E_a$, where $E_a = X_a - \mathbb{E}[X_a]$

$$\Delta^2 = \min_{j \neq k} \| [\mathbf{Q}\mathbf{A}]_{k:} - [\mathbf{Q}\mathbf{A}]_{j:} \|^2 \ge m \times \min_{j \neq k} \| \mathbf{Q}_{k:} - \mathbf{Q}_{j:} \|^2 \quad (\ge 2m \, \lambda_{\min}(\mathbf{Q})^2)$$

$$\Delta^2 = \min_{j \neq k} \|[\mathbf{Q}\mathbf{A}]_{k:} - [\mathbf{Q}\mathbf{A}]_{j:}\|^2 \ge m \times \min_{j \neq k} \|\mathbf{Q}_{k:} - \mathbf{Q}_{j:}\|^2 \quad (\ge 2m \lambda_{\min}(\mathbf{Q})^2)$$

 $L \geq \|\mathbf{Q}\|_{op} \vee 1/m$

Theorem (Giraud and V.('18))

We set $s^2=\Delta^2/L$. If $s^2\gtrsim n/m$ we have $\mathbb{P}[\mathrm{err}(G,\widehat{G})>e^{-cs^2}]\lesssim 1/n^2$

$$\Delta^2 = \min_{j \neq k} \| [\mathbf{Q}\mathbf{A}]_{k:} - [\mathbf{Q}\mathbf{A}]_{j:} \|^2 \ge m \times \min_{j \neq k} \| \mathbf{Q}_{k:} - \mathbf{Q}_{j:} \|^2 \quad (\ge 2m \,\lambda_{\min}(\mathbf{Q})^2)$$

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Theorem (Giraud and V.('18))

We set $s^2 = \Delta^2/L$. If $s^2 \gtrsim n/m$ we have $\mathbb{P}[\operatorname{err}(G, \widehat{G}) > e^{-cs^2}] \lesssim 1/n^2$ if we have enforced $\|\mathbf{B}\|_{op} \leq \frac{K^3}{n} e^{4nL}$.

Assortative case : $\mathbf{Q} = (p-q)\mathbf{I} + q\mathbf{1}\mathbf{1}^T$ and m = n/K

1 $s^2 = 2m(p-q)^2/p$ for $p \ge K/n$. tight constants in Gao et al.('17), Yun and Proutière('14)

2 perfect recovery for

$$\frac{(p-q)^2}{p} \gtrsim \frac{K^2 \vee K \log(n)}{n}$$

Matches Best known polynomial time algorithm condition Chen and Xu('16)

Comments (General ${f Q})$

Exponential decay :

Abbe and Sandon('15) consider the scaling $\mathbf{Q} = \mathbf{Q}_0 \log(n)/n$ for a fixed K. Results not completely comparable.

Perfect recovery : if $\|\mathbf{Q}\|_{op} = O(\min_{j,k} \mathbf{Q}_{jk})$, we recover (up to constant) the optimal condition of Abbe and Sandon('15)

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Other SDP for SBM : Relaxed *K*-means differs from Chen & Xu('16), Hajek et al.('16), Guédon & Vershynin('16), Perry & Wein ('16)...

$$\widetilde{\mathbf{B}} = \operatorname*{arg\,max}_{\mathbf{B} \in \mathcal{C}'} \langle \mathbf{X}, \mathbf{B} \rangle$$

for assortative graphs (diag(Q) > nondiag(Q))

Same arguments, but :

- spectral control requires trimming arguments in the proof
- control of quadratic terms quite messy due to the symmetry of X (peeling, conditionning, ...)

Main message

A corrected convex relaxation of K-means achieves some rate-optimal performances in various settings including (conditional) mixture of sub-Gaussian and (conditional) Stochastic Block Model.

Only tuning Parameter is K

F. Bunea, C. Giraud, M. Royer, N. V. **PECOK : a convex optimization approach to variable clustering**. *Annals of Statistics*. ArXiv:1606.05100

C. Giraud and N.V. **Partial recovery bounds for clustering with the relaxed** K-means. *Mathematical Statistics and Learning* ArXiv:1807.07547

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A corrected convex relaxation of K-means achieves some rate-optimal performances in various settings including (conditional) mixture of sub-Gaussian and (conditional) Stochastic Block Model.

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Merci pour votre attention !

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