# $K$-means: Relaxation and Correction 

## Nicolas Verzelen

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

Clustering individuals w.r.t. features


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 $K$

1 Two clustering Models
$2 K$-means and relaxed $K$-means

3 Corrected $K$-means

4 Partial Recovery bounds
■ subGaussian Mixtures

- Stochastic Block Models


## Mixture of subGaussian variables

## Partition

Partition $G^{*}=\left\{G_{1}^{*}, \ldots, G_{K}^{*}\right\}$ of $\{1, \ldots, n\}$

## Mixture of subGaussian variables (conditional)

$X_{1}, \ldots, X_{n} \in \mathbb{R}^{p}$ are independent with

- $\mathbb{E}\left[X_{a}\right]=\mu_{k}$ if $a \in G_{k}^{*}$
- $\boldsymbol{\Sigma}_{a}^{-1 / 2} X_{a}$ is SubGauss $\left(L^{2} I_{p}\right)$ where $\boldsymbol{\Sigma}_{a}=\operatorname{Cov}\left(X_{a}\right)$ and $L \geq 1$.

The observations are gathered in $\mathbf{X}=\left[X_{1}, \ldots, X_{n}\right] \in \mathbb{R}^{p \times n}$


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Objective : recovering $G^{*}$ from $\mathbf{X}$ ( $\mu$ and $\boldsymbol{\Sigma}$ are unknown but $K$ is known)

## Stochastic Block Model (SBM)

Holland et al(83), Abbe('17),
Let $\mathbf{X}=$ adjacency matrix of an undirected graph $\in\{0,1\}^{n \times n}$.
Let $\mathbf{Q} \in[0,1]_{\text {sym }}^{K \times K}$

## (conditional) SBM

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

$$
\mathbb{P}\left[\mathbf{X}_{a b}=1\right]=\mathbf{Q}_{j k} \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 $\mathbf{A}_{a k}=\mathbf{1}_{a \in G_{k}}$ (or equivalently function $k:[n] \mapsto[K]$ )
is NOT Identifiable. Why?

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

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

$$
\mathbf{B}_{a b}^{*}=\left\{\begin{array}{cl}
\frac{1}{\left|G_{k}^{*}\right|} & \text { if } a \text { and } b \text { belong to the same } G_{k}^{*} \\
0 & \text { else }
\end{array}\right.
$$

Invariant with respect to the group labeling.

## $K$-means criterion

$\widehat{G} \in \arg \min _{G} \operatorname{Crit}(\mathbf{X}, G)$ where

$$
\operatorname{Crit}(\mathbf{X}, G)=\sum_{k=1}^{K} \sum_{a \in G_{k}}\left\|X_{a}-\bar{X}_{G_{k}}\right\|^{2}
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where $\bar{X}_{G_{k}}=\frac{1}{\left|G_{k}\right|} \sum_{a \in G_{k}} X_{a}$

In practice, iterative minimization based on Lloyd's algorithm LLoyd('82).
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Two steps:
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Two caveats :

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

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

## Lemma (Peng \& Wei(07))

The $K$-means minimizer $\widehat{G}$ satisfies

$$
\begin{gathered}
\widehat{\mathbf{B}} \in \arg \min _{\mathbf{B} \in \mathcal{D}}\left\langle-\mathbf{X}^{T} \mathbf{X}, \mathbf{B}\right\rangle, \\
\mathcal{D}:=\left\{\begin{array}{ll} 
& \bullet \mathbf{B} \succcurlyeq 0 \\
\mathbf{B} \in \mathbb{R}^{p \times p}: & \bullet \sum_{a b} \mathbf{B}_{a b}=1, \forall b \\
& \bullet \operatorname{Tr}(\mathbf{B})=K \\
& \bullet \mathbf{B}^{2}=\mathbf{B}
\end{array}\right\}
\end{gathered}
$$

Proof : Perron-Frobenius

Idea: drop the $\mathbf{B}^{2}=\mathbf{B}$ condition.
1 Estimate $\mathbf{B}^{*}$ using the semi-definite program (SDP)

$$
\widehat{\mathbf{B}}=\underset{\mathbf{B} \in \mathcal{C}}{\arg \min }\left\langle-\mathbf{X}^{T} \mathbf{X}, \mathbf{B}\right\rangle
$$

where

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\mathcal{C}:=\left\{\begin{array}{ll} 
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& \bullet \mathbf{B}_{a b} \geqslant 0, \forall a, b \\
& \bullet \operatorname{Tr}(\mathbf{B})=K
\end{array}\right\}
$$

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.


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

## Lemma (Peng \& Wei(07))

Spectral Clustering is equivalent to
1 Estimate B* using the semi-definite program (SDP) $^{*}$

$$
\left.\begin{array}{rl}
\overline{\mathbf{B}} & =\underset{\mathbf{B} \in \overline{\mathcal{C}}}{\arg \min }\left\langle-\mathbf{X}^{T} \mathbf{X}, \mathbf{B}\right\rangle \\
\overline{\mathcal{C}}:=\left\{\mathbf{B} \in \mathbb{R}^{p \times p}:\right. & \bullet 1 \succcurlyeq \mathbf{B} \succcurlyeq 0 \\
\bullet \operatorname{Tr}(\mathbf{B})=K
\end{array}\right\} .\left\{\begin{array}{l}
\end{array}\right.
$$

2 Compute $\widehat{G}$ by distance clustering on the rows of $\overline{\mathbf{B}}$
$\Longrightarrow$ it amounts to dropping the constraints $\mathbf{B} 1=1, \mathbf{B}_{a b} \geqslant 0$ in the former relaxation Proof : 1) $\overline{\mathbf{B}}=\widehat{\mathbf{U}} \widehat{\mathbf{U}}^{T}$
2) $\left(\widehat{\mathbf{U}} \widehat{\mathbf{U}}^{T}\right)_{a} \bullet$ is some orthogonal transformation of $\widehat{\mathbf{U}}_{a} \bullet$.

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



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

## Caveat

## A simple model

Assume that the "points" $X_{a}$ are independent random variables with

$$
\mathbb{E}\left[X_{a}\right]=\mu_{a} \quad \text { and } \quad \operatorname{Tr}\left(\operatorname{Cov}\left(X_{a}\right)\right)=\Gamma_{a}
$$

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

## Expected value at $G$

For a partition $G$ we have

$$
\mathbb{E}\left[\operatorname{Crit}_{K}(G)\right]=\frac{1}{2} \sum_{k} \frac{1}{\left|G_{k}\right|} \sum_{a, b \in G_{k}}\left\|\mu_{a}-\mu_{b}\right\|^{2}+\sum_{a} \Gamma_{a}-\sum_{k} \frac{1}{\left|G_{k}\right|} \sum_{a \in G_{k}} \Gamma_{a}
$$

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

## Caveat (alternative view)

Recall our Minimization Problem : $\left\langle-\mathbf{X}^{T} \mathbf{X}, \mathbf{B}\right\rangle$
sGaussian Mixtures are of the form : $X_{a}=\mathbb{E}\left[X_{a}\right]+E_{a}=$ Information + Noise ,

$$
\mathbb{E}\left[\mathbf{X}^{T} \mathbf{X}\right]=\mathbb{E}[\mathbf{X}]^{T} \mathbb{E}[\mathbf{X}]+\boldsymbol{\Gamma}, \quad \text { where } \boldsymbol{\Gamma}_{a a}=\operatorname{Tr}\left[\operatorname{Cov}\left(E_{a}\right)\right]
$$

## Population $K$-means vs Ideal $K$-means

$$
\begin{aligned}
\mathbf{B}^{\text {pop }} & =\arg \min _{\mathbf{B} \in \mathcal{D}}\left\langle-\mathbb{E}[\mathbf{X}]^{T} \mathbb{E}[\mathbf{X}]-\boldsymbol{\Gamma}, \mathbf{B}\right\rangle \\
\mathbf{B}^{i d} & =\arg \min _{\mathbf{B} \in \mathcal{D}}\left\langle-\mathbb{E}[\mathbf{X}]^{T} \mathbb{E}[\mathbf{X}], \mathbf{B}\right\rangle
\end{aligned}
$$

- Since $\operatorname{Tr}[\mathbf{B}]=K$, we have $\mathbf{B}^{p o p}=\mathbf{B}^{i d}$ when $\boldsymbol{\Gamma}=\gamma \mathbf{I}$.
- For heterogenerous $\boldsymbol{\Gamma}, \mathbf{B}_{a a}^{p o p}$ tends to take large values for large $\boldsymbol{\Gamma}_{a a}$ (it splits wide clusters).

Remark: If we knew the groups, we could estimate $\boldsymbol{\Gamma}=\operatorname{diag}\left(\Gamma_{1}, \ldots, \Gamma_{n}\right)$ by

$$
\widehat{\boldsymbol{\Gamma}}_{a a}=\left\langle X_{a}-X_{n e_{1}(a)}, X_{a}-X_{n e_{2}(a)}\right\rangle
$$

with $n e_{1}(a)$ and $n e_{2}(a)$ 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

Set $U(a, b):=\max _{c, d \in[n] \backslash\{a, b\}}\left|\left\langle X_{a}-X_{b}, \frac{X_{c}-X_{d}}{\left\|X_{c}-X_{d}\right\|}\right\rangle\right|$ and
$\widehat{n e}_{1}(a):=\underset{b \in[n] \backslash\{a\}}{\arg \min } U(a, b)$ and $\widehat{n e}_{2}(a):=\underset{b \in[n] \backslash\left\{a, \widehat{n e}_{1}(a)\right\}}{\arg \min } U(a, b)$
Then, the estimator $\widehat{\Gamma}$ is the diagonal matrix defined by

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$$

Corrected relaxed $K$-means (Bunea et al.('16))
Solve the SDP

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

with

$$
\mathcal{C}:=\left\{\begin{array}{ll} 
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Similarly, one may define a corrected spectral clustering.

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Proportion of misclustered points

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

## Our goal

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

$$
\text { prop. misclustered }=\operatorname{err}\left(\widehat{G}, G^{*}\right) \leq e^{-c s^{2}}
$$

where $s^{2}$ is an appropriate SNR.

Other related goals:

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


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- $\boldsymbol{\Sigma}_{a}^{-1 / 2} X_{a}$ is SubGauss $\left(L^{2} \mathbf{I}_{p}\right)$ where $\boldsymbol{\Sigma}_{a}=\operatorname{cov}\left(X_{a}\right)$

We set

$$
\Delta^{2}=\min _{j \neq k}\left\|\mu_{k}-\mu_{j}\right\|^{2}, \quad \sigma^{2}=L^{2} \max _{k}\left|\boldsymbol{\Sigma}_{k}\right|_{o p} \quad \text { and } \quad R_{\boldsymbol{\Sigma}}=\max _{k} \frac{\left|\boldsymbol{\Sigma}_{k}\right|_{F}^{2}}{\left|\boldsymbol{\Sigma}_{k}\right|_{o p}^{2}},
$$

and define the SNR

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

where $m$ denotes the size of the smallest cluster.

Simplification : $K=2,\left|G_{1}^{*}\right|=\left|G_{-1}^{*}\right|=n / 2, \boldsymbol{\Sigma}_{1}=\boldsymbol{\Sigma}_{-1}=\sigma^{2} \mathbf{I}_{p}, \mu_{-1}=-\mu_{1}$.
Simplified Model $1: \mu_{1}$ is known. Bayes Classifier achieves :

$$
\mathbb{E}\left[\operatorname{err}\left(\widehat{G}, G^{*}\right)\right]=2 \mathbb{P}\left[\mathcal{N}\left(0, \sigma^{2}\right)>\left\|\mu_{1}\right\|\right] \leq 2 \exp \left[-\frac{\Delta^{2}}{8 \sigma^{2}}\right]
$$

Simplified Model 2: $\mu_{1}$ 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 : $\widehat{h}(x)=\operatorname{sign}\left(\left\langle\frac{1}{n} \sum_{a=1}^{n} Z_{a} X_{a}, x\right\rangle\right)$ :

- achieves the rate $e^{-c \Delta^{2} / \sigma^{2}}$ if $\frac{\Delta^{2}}{\sigma^{2}} \gtrsim 1 \vee \frac{p}{n}$.
- achieves the rate $e^{-c n \Delta^{4} /\left(p \sigma^{4}\right)}$ 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.

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

## Theorem (Giraud and V. ('18))

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

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

## Remarks :

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

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2 perfect recovery for $s^{2} \gtrsim \log (n) \vee(n / m) \quad=\log (n) \vee K$
Dependency in $K$ is suboptimal.
Vempala and Wang('04) $\rightsquigarrow s^{2} \gtrsim \log (n) \vee \sqrt{K \log (n)}$ when $n \gg p^{3}$.
3 Do not cover the case where the proportion of error is $\geq e^{-c^{\prime \prime} K}$.

Mild price for $\boldsymbol{\Gamma}$ estimation: $\frac{\left\|\boldsymbol{\Sigma}_{k}\right\|_{o p} \operatorname{Tr}\left(\boldsymbol{\Sigma}_{k}\right)}{\left\|\boldsymbol{\Sigma}_{k}\right\|_{F}^{2}} \lesssim \frac{n}{\log (n)}$

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Without correction, additional assumption is required :

$$
\Delta^{2} \gtrsim \frac{\max \boldsymbol{\Gamma}_{a}-\min \boldsymbol{\Gamma}_{a}}{m}
$$

For a balanced Partition, it amounts to

$$
\Delta^{2} \gtrsim \sigma^{2} K\left(1 \vee \sqrt{\frac{R_{\boldsymbol{\Sigma}}}{n}} \vee \frac{\max _{k} \operatorname{tr}\left[\boldsymbol{\Sigma}_{k}\right]-\min _{k} \operatorname{tr}\left[\boldsymbol{\Sigma}_{k}\right]}{n}\right] .
$$

Simple Versions: All $\left\|\mu_{i}-\mu_{j}\right\|_{2}$ are equal
Step 1 : $\left|\widehat{\mathbf{B}}-\mathbf{B}^{*}\right|_{1}$ small implies that $\operatorname{err}(\widehat{G}, G)$ is small.
New Objective : Show that $\left\langle\mathbf{X}^{T} \mathbf{X}-\widehat{\boldsymbol{\Gamma}}, \mathbf{B}^{*}-\mathbf{B}\right\rangle>0$ as long as $\left|\mathbf{B}^{*}-\mathbf{B}\right|_{1}$ is not small

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

We focus on the two first terms
Signal Term : $\left\langle\mathbf{A} \mu \mu^{T} \mathbf{A}^{T}, \mathbf{B}^{*}-\mathbf{B}\right\rangle=\frac{1}{4} \Delta^{2}\left|\mathbf{B}^{*}-\mathbf{B}^{*} \mathbf{B}\right|_{1}$

## Control of the quadratic term : $\left\langle\mathbf{E}^{T} \mathbf{E}-\mathbf{\Gamma}, \mathbf{B}^{*}-\mathbf{B}\right\rangle$

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

B* is projection operator that averages over element of the same group.
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Step 3 : Control of the Projection Along $\operatorname{Im}\left(\mathbf{B}^{*}\right)$

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

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

## Control of the quadratic term : $\left\langle\mathbf{E}^{T} \mathbf{E}-\mathbf{\Gamma}, \mathbf{B}^{*}-\mathbf{B}\right\rangle$

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$$

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

Step 4 : Control of $\left\langle\mathbf{B}^{*}\left(\mathbf{E}^{T} \mathbf{E}-\boldsymbol{\Gamma}\right), \mathbf{B}^{*}-\mathbf{B}\right\rangle$.
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 $\mathbf{A}_{(1)} \geq \mathbf{A}_{(2)} \geq \ldots$
Control of the order statistics $\mathbf{B}^{*}\left(\mathbf{E}^{T} \mathbf{E}-\mathbf{\Gamma}\right)$ by Hanson-Wright inequality + Union bound

## (conditional) SBM

Assume that the graph is generated by a SBM with $\mathbf{Q}_{j k}=$ probability of connection between nodes of groups $j$ and $k$.
Let $\mathbf{X}=$ adjacency matrix of the graph $\in\{0,1\}^{n \times n}$.

$$
\underline{\text { For } a \in G_{k}^{*}: \quad X_{a}=[\mathbf{Q A}]_{k:}-\mathbf{Q}_{k k} e_{a}+E_{a}, \quad \text { where } \quad E_{a}=X_{a}-\mathbb{E}\left[X_{a}\right]}
$$

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

$$
\begin{gathered}
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L \geq\|\mathbf{Q}\|_{o p} \vee 1 / m
\end{gathered}
$$

## Theorem (Giraud and $V$. (18))

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

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## Theorem (Giraud and V. (18))

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

Assortative case : $\mathbf{Q}=(p-q) \mathbf{I}+q 11^{T}$ and $m=n / K$
$1 s^{2}=2 m(p-q)^{2} / p$ for $p \geq K / n$. 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 $\mathrm{Xu}($ '16)

## Comments (General 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 $\|\mathbf{Q}\|_{o p}=O\left(\min _{j, k} \mathbf{Q}_{j k}\right)$, 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)...

$$
\widetilde{\mathbf{B}}=\underset{\mathbf{B} \in \mathcal{C}^{\prime}}{\arg \max }\langle\mathbf{X}, \mathbf{B}\rangle
$$

for assortative graphs $(\operatorname{diag}(\mathbf{Q})>$ nondiag $(\mathbf{Q}))$

Same arguments, but :

- spectral control requires trimming arguments in the proof
- control of quadratic terms quite messy due to the symmetry of $\mathbf{X}$ (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

## 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.

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## Merci pour votre attention!

E. Abbe.

Community detection and stochastic block models : recent developments.
ArXiv e-prints, March 2017.
易
Pranjal Awasthi, Moses Charikar, Ravishankar Krishnaswamy, and Ali Kemal Sinop.
The Hardness of Approximation of Euclidean k-means.
arXiv preprint arXiv :1502.03316, 2015.
Emmanuel Abbe and Colin Sandon.
Community Detection in General Stochastic Block Models: Fundamental Limits and Efficient Algorithms for Recovery.
In
Proceedings of the 2015 IEEE 56th Annual Symposium on Foundations of Computer Scie FOCS '15, pages 670-688, Washington, DC, USA, 2015. IEEE Computer Society.

Yudong Chen and Jiaming Xu.
Statistical-computational tradeoffs in planted problems and submatrix localization with a growing number of clusters and submatrices.
Journal of Machine Learning Research, 17(27) :1-57, 2016.
Y. Fei and Y. Chen.

Exponential error rates of SDP for block models : Beyond Grothendieck's inequality.
ArXiv e-prints, 2017.
Y. Fei and Y. Chen.

Hidden Integrality of SDP Relaxation for Sub-Gaussian Mixture Models.
ArXiv e-prints, March 2018.
R- Chao Gao, Zongming Ma, Anderson Y. Zhang, and Harrison H. Zhou. Achieving Optimal Misclassification Proportion in Stochastic Block Models.
J. Mach. Learn. Res., 18(1) :1980-2024, January 2017.


Olivier Guédon and Roman Vershynin.
Community detection in sparse networks via Grothendieck's inequality. arXiv preprint arXiv :1411.4686, 2014.

Paul W Holland, Kathryn Blackmond Laskey, and Samuel Leinhardt.
Stochastic blockmodels: First steps.
Social networks, 5(2) :109-137, 1983.

B. Hajek, Y. Wu, and J. Xu.

Semidefinite Programs for Exact Recovery of a Hidden Community. ArXiv e-prints, February 2016.
S. Lloyd.

Least Squares Quantization in PCM.
IEEE Trans. Inf. Theor., 28(2) :129-137, September 1982.
Mohamed Ndaoud.
Sharp optimal recovery in the Two Component Gaussian Mixture Model.
arXiv e-prints, page arXiv :1812.08078, Dec 2018.
Jiming Peng and Yu Wei.
Approximating K-means-type Clustering via Semidefinite Programming. SIAM J. on Optimization, 18(1) :186-205, February 2007.
A. Perry and A. S. Wein.

A semidefinite program for unbalanced multisection in the stochastic block model.
ArXiv e-prints, July 2015.


Santosh Vempala and Grant Wang.
A spectral algorithm for learning mixture models.
Journal of Computer and System Sciences, 68(4) :841-860, 2004.
Special Issue on FOCS 2002.

Se-Young Yun and Alexandre Proutière.
Accurate Community Detection in the Stochastic Block Model via Spectral Algorithms. CoRR, abs/1412.7335, 2014.

