Probably certifiably correct k-means clustering

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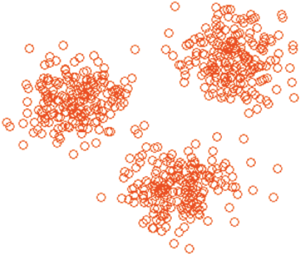
The k-means problem

Given a point cloud, partition the points into concentrated clusters



k-means objective:

$$\sum_{t=1}^{k} \sum_{i \in C_t} \left\| x_i - \frac{1}{|C_t|} \sum_{j \in C_t} x_j \right\|^2$$

- NP-hard to minimize in general
- Lloyd's algorithm often works, but no optimality certificate

An SDP relaxation

Taking $D_{ij} := \|x_i - x_j\|^2$, then

$$\sum_{t=1}^{k} \sum_{i \in C_t} \left\| x_i - \frac{1}{|C_t|} \sum_{j \in C_t} x_j \right\|^2 = \frac{1}{2} \operatorname{Tr}\left(D \sum_{t=1}^{k} \frac{1}{|C_t|} 1_{C_t} 1_{C_t}^\top \right)$$

Peng, Wei, SIAM J. Optim., 2007

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Proof:

$$\begin{aligned} \operatorname{Tr}(D 1_{C_t} 1_{C_t}^\top) &= \sum_{i \in C_t} \sum_{j \in C_t} \|x_i - x_j\|^2 \\ &= \sum_{i \in C_t} \sum_{j \in C_t} \left\| (x_i - c_t) - (x_j - c_t) \right\|^2 \\ &= 2|C_t| \sum_{i \in C_t} \|x_i - c_t\|^2 \end{aligned}$$

Divide by $2|C_t|$ and add. $\square$

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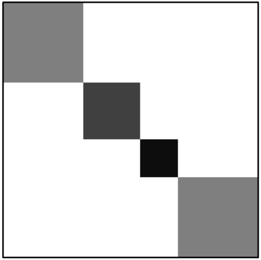

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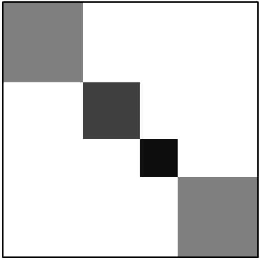

Relax to SDP:

$$\begin{aligned} \text{minimize} \quad & \operatorname{Tr}(DX) \\ \text{subject to} \quad & \operatorname{Tr}(X) = k \\ & X1 = 1 \\ & X \geq 0 \\ & X \succeq 0 \end{aligned}$$

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Faster certified clustering?

SDP solvers are polytime, but slow

SDP clusters 64 points in 20 sec, Lloyd takes 0.001 sec

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Probably certifiably correct algorithm

- Oracle provides k-means-optimal solution whp
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How is this possible?

- Tight convex relaxation
- Clever computation of dual certificate

Collaborators

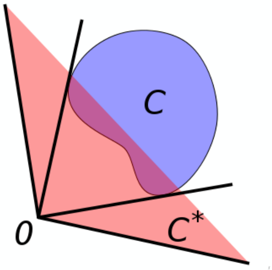
Takayuki Iguchi
AFIT

Jesse Peterson
AFIT

Soledad Villar
UT Austin

Preliminaries

Dual cone: $C^* := \{x : \langle x, y \rangle \geq 0 \;\; \forall y \in C\}$



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Primal program:

$$\begin{aligned} \max \quad & \langle c, x\rangle \\ \text{s.t.} \quad & b - Ax \in L \\ & x \in K \end{aligned}$$

Dual program:

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Weak duality: $\langle b - Ax, y \rangle \geq 0$, $\langle x, A^\top y - c \rangle \geq 0$

$$\implies \qquad \langle c, x \rangle \leq \langle x, A^\top y \rangle = \langle Ax, y \rangle \leq \langle b, y \rangle$$

Strong duality: $\langle c, x_{\mathrm{opt}} \rangle = \langle b, y_{\mathrm{opt}} \rangle$ "dual certificate"

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Complementary slackness

x is primal-opt and y is dual-opt if and only if

- x is primal feasible
- y is dual feasible
- $\langle b - Ax, y \rangle = \langle x, A^\top y - c \rangle = 0$

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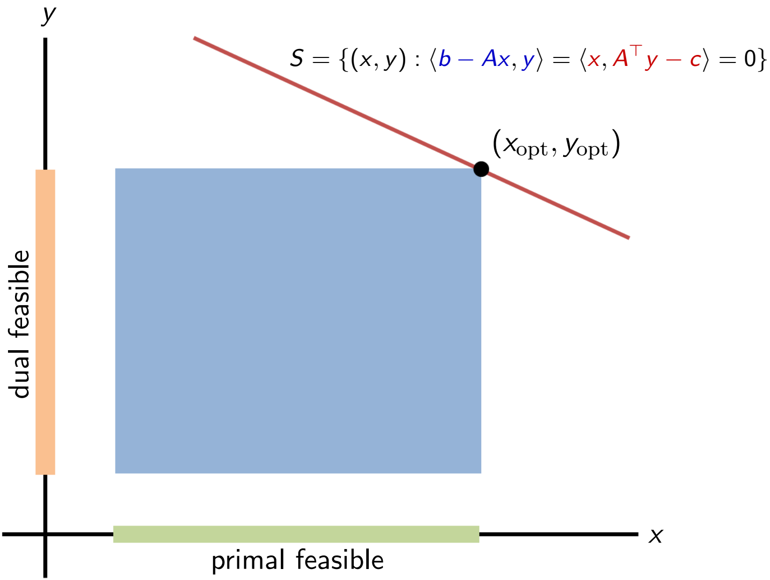
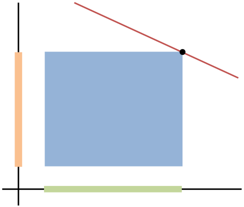


The big idea (Afonso Bandeira)

Task: Given x_{opt}, quickly find y_{opt}

Method:

1. Check that x_{opt} is primal feasible
2. Find y such that $(x_{\mathrm{opt}}, y) \in S$
3. Check that y is dual feasible



Bandeira, `arXiv:1509.00824`

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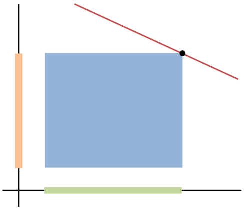

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Example: Minimum bisection in stochastic block model

- Easy to find **unique** y such that $(x_{\mathrm{opt}}, y) \in S$
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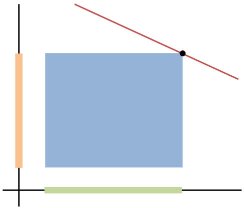

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Problem: y is **not unique** in the case of k-means
(Choice of y is an art form, "optimal" choice remains open)

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A small technicality

Subproblem in checking dual feasibility:

Is $\operatorname{span}(v)$ **the unique leading eigenspace of** A**?**

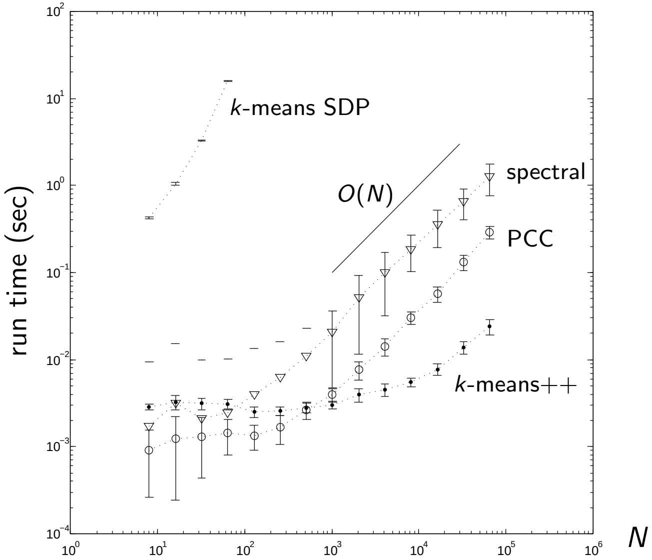
Fast solution: Power method from random initialization

Report $1-\eta$ confidence after $O(\log(1/\eta))$ power iterations

Open problem: Remove the possibility of "false certificates"

Iguchi, M., Peterson, Villar, `arXiv:1509.07983`

It works, and it's fast!



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Guarantee for random problem instances

$(\mathcal{D}, \gamma, n)$-**stochastic ball model**

- $\mathcal{D}$ = rotation-invariant distribution over unit ball in $\mathbb{R}^m$
- $\gamma_1, \ldots, \gamma_k$ = ball centers in $\mathbb{R}^m$
- Draw $r_{t,1}, \ldots, r_{t,n}$ i.i.d. from $\mathcal{D}$ for each $i \in \{1, \ldots, k\}$
- $x_{t,i} = \gamma_t + r_{t,i}$ = ith point from cluster t

When does the PCC method certify the planted solution whp?

Nellore, Ward, `arXiv:1309.3256`

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When does the PCC method certify the planted solution whp?

Theorem

PCC certifies the planted solution under $(\mathcal{D}, \gamma, n)$-SBM w.p. $1 - e^{-\Omega_{\mathcal{D},\gamma}(n)}$ if

$$\min_{i \neq j} \|\gamma_i - \gamma_j\| \geq 2 + \frac{k^2}{m}$$

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When does SDP recover planted clustering?

Corollary

SDP recovers the planted solution under $(\mathcal{D}, \gamma, n)$-SBM w.p. $1 - e^{-\Omega_{\mathcal{D},\gamma}(n)}$ if

$$\min_{i \neq j} \|\gamma_i - \gamma_j\| \geq \min\left\{2 + \frac{k^2}{m},\ 2\sqrt{2}(1 + \frac{1}{\sqrt{m}})\right\}$$

Bounds from different choices of dual certificate (art form)

Appears loose in the small-m regime

What is the best bound?

Awasthi, Bandeira, Charikar, Krishnaswamy, Villar, Ward, Proc. ITCS, 2015

Iguchi, M., Peterson, Villar, arXiv:1509.07983

When does SDP recover planted clustering?

Natural conjecture: SDP recovers whp provided $\min_{i \neq j} \|\gamma_i - \gamma_j\| > 2$

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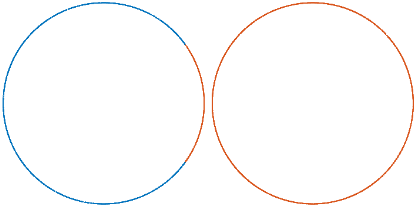

The planted clustering is not k-means-optimal!

Open problem: Necessary separation for two $(m-1)$-spheres?

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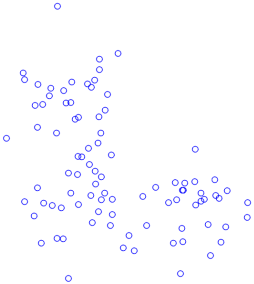
What about outliers?

SBM allows for SDP tightness, but is the model good?



SDP guarantees for more realistic data? **(see Soledad's talk)**

Open problems

- Derandomize leading eigenspace certifier
- Optimal bounds for k-means under SBM
- How to pick k?

Questions?

A note on probably certifiably correct algorithms
A. S. Bandeira
arXiv:1509.00824

Probably certifiably correct *k*-means clustering
T. Iguchi, D. G. Mixon, J. Peterson, S. Villar
arXiv:1509.07983

Also, google **short fat matrices** for my research blog