Clustering

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COMS 4772

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Finitely representing large sets

Let (\mathcal{X}, ρ) be a metric space.

▶ I.e., ρ : $\mathcal{X} \times \mathcal{X} \to \mathbb{R}_+$ is symmetric, non-negative (with $\rho(x,y) = 0$ iff x = y), and satisfies triangle inequality.

Goal: given a set $S \subset \mathcal{X}$, find a set $C \subset \mathcal{X}$ ("centers") that

- has small cardinality, and
- "represents" the set S well (as measured by a cost function).

Covering / net formulations

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k-center clustering

- ▶ Fix the cardinality $k \in \mathbb{N}$ allowed for C.
- ► Cost function:

$$cost_{\infty}(S, C) := \max_{\mathbf{x} \in S} \rho(\mathbf{x}, C),$$

where $\rho(\mathbf{x}, C) := \min_{\mathbf{y} \in C} \rho(\mathbf{x}, \mathbf{y})$.

- ▶ Determines ε in ε -net criterion.
- ▶ NP-hard optimization problem.

Farthest-first traversal (Gonzalez, 1985)

- ▶ Input: set $S \subset \mathcal{X}$.
- ▶ Let y_1 be any point in S.
- ▶ For t = 2, 3, ...:
 - Let y_t be a point in S farthest from all previous y_i :

$$\label{eq:max_problem} \mbox{\textbf{\emph{y}}}_t \; \in \; \arg\max_{\mbox{\textbf{\emph{x}}} \in \mbox{\textbf{\emph{S}}}} \rho \big(\mbox{\textbf{\emph{x}}}, \{\mbox{\textbf{\emph{y}}}_1, \mbox{\textbf{\emph{y}}}_2, \dots, \mbox{\textbf{\emph{y}}}_{t-1}\} \big) \,.$$

▶ **Theorem**. For any k, cost of $\widehat{C} := \{y_1, y_2, \dots, y_k\}$ is at most twice the cost of every C with $|C| \le k$.

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Approximation analysis of farthest-first

▶ Let $r_i := \rho(\mathbf{y}_{i+1}, \{\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_i\})$, so

$$r_k = \rho(\mathbf{y}_{k+1}, \widehat{C}) = \max_{\mathbf{x} \in S} \rho(\mathbf{x}, \widehat{C}) = \cot(S, \widehat{C}).$$

- ▶ Pairwise distances among $\{y_1, y_2, ..., y_{i+1}\}$ are at least r_i .
 - $So r_1 \ge r_2 \ge \cdots \ge r_k.$
- ightharpoonup Consider any set of at most k representatives C.
- At least two points in $\{y_1, y_2, \dots, y_{k+1}\}$ have same closest representative in C.
 - ▶ Say they are y_i and y_i , and they are represented by $z \in C$.
 - By triangle inequality,

$$2 \cdot \mathsf{cost}_{\infty}(S, C) \geq \rho(\mathbf{y}_i, \mathbf{z}) + \rho(\mathbf{y}_i, \mathbf{z}) \geq \rho(\mathbf{y}_i, \mathbf{y}_i) \geq r_k$$

• So
$$\mathsf{cost}_{\infty}(S,\widehat{C}) = r_k \leq 2 \cdot \mathsf{cost}_{\infty}(S,C)$$
.

ε -nets

▶ Suppose we run farthest-first traversal to pick $y_1, y_2, ...$, and stop as soon as

$$r_k = \cos(S, \{y_1, y_2, \dots, y_k\}) \leq \varepsilon.$$

- ▶ Then $\widehat{C}:=\{\pmb{y}_1,\pmb{y}_2,\dots,\pmb{y}_k\}$ satisfies size of smallest ε -net $\leq |\widehat{C}| \leq$ size of smallest ε /2-net.
- ▶ Size of smallest ε -net is called *covering number of S* (at scale ε , with respect to ρ metric).

Set cover

▶ **Goal**: given set S, family of subsets $\mathcal{F} := \{S_i : i \in \mathcal{I}\} \subseteq 2^S$, pick $S_{i_1}, S_{i_2}, \ldots, S_{i_k}$, with k as small as possible, that cover S:

$$\bigcup_{j=1}^k S_{i_j} = S.$$

- ▶ (Can assume $\bigcup_{i \in \mathcal{I}} S_i = S_i$.)
- ► Example:
 - $S \subseteq \mathcal{X}$ for some metric space (\mathcal{X}, ρ) .
 - ▶ $\mathcal{F} = \{B(c, \varepsilon) \cap S : c \in S\}$, where $B(c, r) := \{x \in \mathcal{X} : \rho(x, c) \le r\}$ is ball of radius r around c.

Greedy algorithm

- ▶ Assume *S* has cardinality $n < \infty$.
- ▶ Having already selected $S_{i_1}, S_{i_2}, \ldots, S_{i_t}$, we next select

$$i_{t+1} \in \underset{i \in \mathcal{I}}{\operatorname{arg\,max}} \left| S_i \cap \left(S \setminus \bigcup_{j=1}^t S_{i_j} \right) \right|.$$

(Halt when S is covered.)

▶ **Theorem**. If there is a cover of size k, then greedy finds a cover of size $k(1 + \ln(n/k))$.

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Analysis of greedy algorithm (Johnson, 1974)

- ▶ Suppose $S_{i_1^{\star}}, S_{i_2^{\star}}, \dots, S_{i_k^{\star}}$ covers S.
- After t steps of greedy, we have picked $S_{i_1}, S_{i_2}, \ldots, S_{i_t}$.
 - ▶ Let $n_t := |S \setminus \bigcup_{j=1}^t S_{i_j}|$ be the number of points in S not covered after t steps.
 - lacksquare We know $S_{i_1^\star}, S_{i_2^\star}, \ldots, S_{i_k^\star}$ would cover all n_t points.
 - So there is one of them covers at least n_t/k of the n_t points.
 - Greedy does at least well with its choice i_{t+1} .
- Starting with $n_0 = n$, we have

$$n_{t+1} \leq \left(1 - \frac{1}{k}\right) n_t.$$

- ▶ So $n_t \le k$ for $t \ge k \ln(n/k)$.
- ▶ After this, just need *k* more sets to cover remaining points.
- ▶ Total of $k(1 + \ln(n/k))$ sets.

Average cost formulations

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k-medians and k-means cost functions

- ightharpoonup Instead of requiring representatives close to every point in S, just require representatives close to random point in S.
- ► Some common cost functions:
 - ► *k*-medians: $cost(S, C) = \sum_{x \in S} \rho(x, C)$. ► *k*-means: $cost(S, C) = \sum_{x \in S} \rho(x, C)^2$.

k-means

- - $cost(S, C) = \sum_{\mathbf{x} \in S} \min_{\mathbf{y} \in C} \|\mathbf{x} \mathbf{y}\|_{2}^{2}.$
- NP-hard to approximate within some constant factor c > 1 (Awasthi et al, 2015).
- Easy cases:
 - ▶ d = 1: dynamic programming in time $O(n^2k)$.
 - k = 1: bias-variance decomposition

$$\sum_{\mathbf{x} \in S} \|\mathbf{x} - \mathbf{y}\|_{2}^{2} = |S| \cdot \|\mathbf{y} - \text{mean}(S)\|_{2}^{2} + \sum_{\mathbf{x} \in S} \|\mathbf{x} - \text{mean}(S)\|_{2}^{2}$$

implies solution is mean(S).

▶ Approximation schemes available when d = O(1) or k = O(1).

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General case

- ▶ Notation: for $C = \{y_1, y_2, \dots, y_k\}$,
 - $C(x) := \arg\min_{y \in C} ||x y||_2^2$, ties broken using some fixed rule.
 - $S_i^C = S_i := \{ x \in S : C(x) = y_i \} \text{ for each } i = 1, 2, ..., k.$
- ► Improving *C*:

$$cost(S, C) = \sum_{i=1}^{k} cost(S_i, C)$$

$$= \sum_{i=1}^{k} cost(S_i, \mathbf{y}_i)$$

$$\geq \sum_{i=1}^{k} cost(S_i, mean(S_i))$$

$$\geq \sum_{i=1}^{k} cost(S_i, \{mean(S_j) : j = 1, 2, ..., k\})$$

$$= cost(S, \{mean(S_i) : j = 1, 2, ..., k\}).$$

Local search algorithm (Lloyd, 1982)

- ▶ Start with $C = \{y_1, y_2, \dots, y_k\}$; repeat:
 - ▶ Partition S into $S_1, S_2, ..., S_k$ using C.
 - ► Set $C := \{ mean(S_i) : i = 1, 2, ..., k \}.$
- ▶ Alternative: start with partition of S into S_1, S_2, \ldots, S_k .
- Cost is non-increasing.
- ▶ Eventually halts, because there are only $O(n^{dk^2})$ ways to partition n points in \mathbb{R}^d with k Voronoi cells.
 - Could take $2^{\Omega(n)}$ iterations (when $k = \Theta(n)$), but atypical.
- ► How good is final solution?
 - Depends on initialization.
 - ► Could be arbitrarily worse than optimal.

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Bad case for Lloyd's algorithm

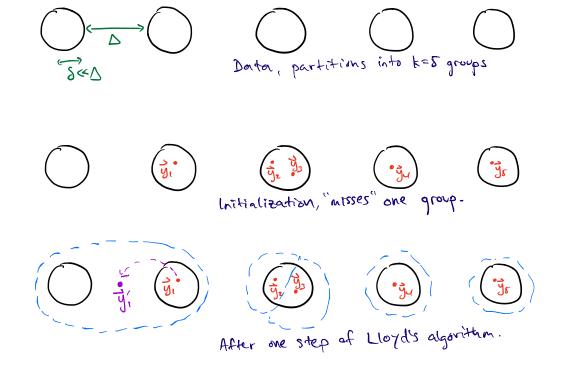


Figure 1: Bad case for Lloyd's algorithm

Aside: dimension reduction

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Another look at bias-variance

$$\sum_{\mathbf{x} \in S} \|\mathbf{x} - \mathbf{y}\|_2^2 = \|S| \cdot \|\mathbf{y} - \text{mean}(S)\|_2^2 + \sum_{\mathbf{x} \in S} \|\mathbf{x} - \text{mean}(S)\|_2^2.$$

Now averaging over $y \in S$:

$$\frac{1}{|S|} \sum_{\mathbf{x}, \mathbf{y} \in S} \|\mathbf{x} - \mathbf{y}\|_{2}^{2} = \sum_{\mathbf{y} \in S} \|\mathbf{y} - \text{mean}(S)\|_{2}^{2} + \sum_{\mathbf{x} \in S} \|\mathbf{x} - \text{mean}(S)\|_{2}^{2}$$
$$= 2 \sum_{\mathbf{x} \in S} \|\mathbf{x} - \text{mean}(S)\|_{2}^{2}.$$

Dimension reduction for k-means

Let S be partitioned into S_1, S_2, \ldots, S_k by $C = \{y_1, y_2, \ldots, y_k\}$.

- ▶ Assume $y_i = \text{mean}(S_i)$ (i.e., C is locally optimal).
- ► Bias-variance implies

$$cost(S, C) = \sum_{i=1}^{k} \sum_{\mathbf{x} \in S_i} \|\mathbf{x} - mean(S_i)\|_2^2$$
$$= \sum_{i=1}^{k} \frac{1}{2|S_i|} \sum_{\mathbf{x}, \mathbf{x} \in S_i} \|\mathbf{x} - \mathbf{x}'\|_2^2,$$

so cost only depends on pairwise distances between data.

- ▶ Can thus reduce dimension (using JL) to $O(\log(n)/\varepsilon^2)$ and preserve cost of all locally-optimal solutions up to $1 \pm \varepsilon$ factor.
- Also implies that we cannot expect $poly(n, k, 2^{O(d)})$ -time exact algorithm for k-means.

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D^2 sampling

D^2 sampling

Problem. Lloyd's algorithm requires good initialization.

 D^2 sampling / k-means++ (Arthur and Vassilvitskii, 2007)

- ▶ Pick \mathbf{Y}_1 u.a.r. from S, and set $C_1 := \{\mathbf{Y}_1\}$.
- ▶ For t = 2, 3, ...:
 - ▶ Pick $\boldsymbol{Y}_t \sim p_t$, where

$$p_t(\mathbf{y}) = \frac{\mathsf{cost}(\{\mathbf{y}\}, C_{t-1})}{\mathsf{cost}(S, C_{t-1})}$$
 for each $\mathbf{y} \in S$.

Theorem.

$$\mathbb{E} \cot(S, C_k) \leq O(\log k) \cdot \min_{C \subseteq \mathbb{R}^d : |C| \leq k} \cot(S, C).$$

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Analysis of the first center selection

- Let $C^* := \{\mu_1, \mu_2, \dots, \mu_k\}$ be optimal solution, and let A_1, A_2, \dots, A_k be partitioning of S with respect to C^* .
- First analyze Y_1 , which is distributed uniformly at random in S.
- Claim.

$$\mathbb{E}\left[\mathsf{cost}(A_i, C_1) \mid \{\mathbf{Y}_1 \in A_i\}\right] = 2 \mathsf{cost}(A_i, C^*).$$

Proof. By bias-variance,

$$\mathbb{E}\left[\sum_{\mathbf{x}\in A_{i}}\|\mathbf{x}-\mathbf{Y}_{1}\|_{2}^{2} \mid \{\mathbf{Y}_{1}\in A_{i}\}\right]$$

$$=\mathbb{E}\left[\sum_{\mathbf{x}\in A_{i}}\|\mathbf{x}-\boldsymbol{\mu}_{i}\|_{2}^{2} + |A_{i}| \cdot \|\mathbf{Y}_{1}-\boldsymbol{\mu}_{i}\|_{2}^{2} \mid \{\mathbf{Y}_{1}\in A_{i}\}\right]$$

$$=2\sum_{\mathbf{x}\in A_{i}}\|\mathbf{x}-\boldsymbol{\mu}_{i}\|_{2}^{2}. \quad \Box$$

▶ (Lose factor of two by restricting centers to data points.)

Selection of subsequent centers

- ▶ Now consider Y_t for t > 1 (conditional on C_{t-1}).
- ▶ Distribution of Y_t not necessarily uniform in S.
 - ▶ Points farther from C_{t-1} get higher weight in p_t .
- ▶ Write, for $\mathbf{y} \in A_i$,

$$p_t(\mathbf{y}) = \underbrace{\frac{\cot(\{\mathbf{y}\}, C_{t-1})}{\cot(A_i, C_{t-1})}}_{=: p_t(\mathbf{y}|A_i)} \cdot \underbrace{\frac{\cot(A_i, C_{t-1})}{\cot(S, C_{t-1})}}_{=: p_t(A_i)}.$$

▶ Claim (non-uniformity bound). For $y \in A_i$,

$$p_t(\boldsymbol{y} \mid A_i) \leq \frac{2}{|A_i|} \left(1 + \frac{\cos(A_i, \{\boldsymbol{y}\})}{\cos(A_i, C_{t-1})}\right).$$

Claim (cost bound).

$$\mathbb{E}\left[\operatorname{cost}(A_i, C_{t-1} \cup \{\boldsymbol{Y}_t\}) \mid \{\boldsymbol{Y}_t \in A_i\}, C_{t-1}\right] \leq 8 \operatorname{cost}(A_i, C^*).$$

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Non-uniformity bound

Proof of non-uniformity bound.

- ► For any $\mathbf{x} \in A_i$, $\cos(\{\mathbf{y}\}, C_{t-1}) \leq \cos(\{\mathbf{y}\}, \{C_{t-1}(\mathbf{x})\}) = \|\mathbf{y} C_{t-1}(\mathbf{x})\|_2^2 .$
- By triangle inequality,

$$cost(\{\boldsymbol{y}\}, C_{t-1}) \leq 2(\|\boldsymbol{x} - C_{t-1}(\boldsymbol{x})\|_2^2 + \|\boldsymbol{x} - \boldsymbol{y}\|_2^2).$$

▶ Now average with respect to $x \in A_i$:

$$cost(\{y\}, C_{t-1}) \leq \frac{2}{|A_i|} cost(A_i, C_{t-1}) + \frac{2}{|A_i|} cost(A_i, \{y\}).$$

So

$$p_t(\boldsymbol{y} \mid A_i) = \frac{\operatorname{cost}(\{\boldsymbol{y}\}, C_{t-1})}{\operatorname{cost}(A_i, C_{t-1})} \leq \frac{2}{|A_i|} \left(1 + \frac{\operatorname{cost}(A_i, \{\boldsymbol{y}\})}{\operatorname{cost}(A_i, C_{t-1})}\right). \quad \Box$$

Cost bound

Proof of cost bound.

Expected cost:

$$\sum_{\boldsymbol{y}\in A_i} p_t(\boldsymbol{y}\mid A_i) \cdot \mathsf{cost}(A_i, C_{t-1} \cup \{vy\})$$

▶ Using non-uniformity bound on $p_t(\cdot \mid A_i)$:

$$\leq \sum_{\boldsymbol{y} \in A_i} \frac{2}{|A_i|} \left(1 + \frac{\mathsf{cost}(A_i, \{\boldsymbol{y}\})}{\mathsf{cost}(A_i, C_{t-1})} \right) \cdot \mathsf{cost}(A_i, C_{t-1} \cup \{\boldsymbol{y}\})$$

▶ Using $cost(A_i, C_{t-1} \cup \{y\}) \le min\{cost(A_i, \{y\}), cost(A_i, C_{t-1})\}$:

$$\leq \frac{4}{|A_i|} \sum_{\mathbf{y} \in A_i} \operatorname{cost}(A_i, \{\mathbf{y}\}) = 8 \operatorname{cost}(A_i, \operatorname{mean}(A_i))$$
$$= 8 \operatorname{cost}(A_i, C^*).$$

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Cost of uncovered clusters

So for any t,

$$\mathbb{E}\left[\operatorname{cost}(A_i, C_{t-1} \cup \{\boldsymbol{Y}_t\}) \mid \{\boldsymbol{Y}_t \in A_i\}, C_{t-1}\right] \leq 8 \operatorname{cost}(A_i, C^*).$$

- **Problem**: some Y_t land in already covered A_i .
- ▶ Define "good" and "bad" points:

$$\text{good (covered):} \quad G_t \ := \ \bigcup_{i:A_i \cap C_t \neq \emptyset} A_i \,, \quad g_t \ := \ \left| \left\{ i:A_i \cap C_t \neq \emptyset \right\} \right|,$$

bad (uncovered):
$$B_t := \bigcup_{i:A_i \cap C_t = \emptyset} A_i$$
, $b_t := |\{i:A_i \cap C_t = \emptyset\}|$.

And define potential function

$$\Phi_t := \frac{t - g_t}{b_t} \cos(B_t, C_t).$$

▶ Since $g_k + b_k = k$,

$$cost(S, C_k) = cost(G_k, C_k) + \Phi_k.$$

Change in uncovered clusters potential

Claim (proof omitted).

$$\mathbb{E} \big[\Phi_{t+1} - \Phi_t \mid \{ \boldsymbol{Y}_{t+1} \in B_t \}, \ C_t \big] \leq 0, \\ \mathbb{E} \big[\Phi_{t+1} - \Phi_t \mid \{ \boldsymbol{Y}_{t+1} \in G_t \}, \ C_t \big] \leq \frac{\cos(B_t, C_t)}{b_t}.$$

Using this claim, it follows that

$$\mathbb{E}\left[\Phi_{t+1} - \Phi_{t} \mid C_{t}\right] \leq \mathbb{P}(\boldsymbol{Y}_{t+1} \in G_{t} \mid C_{t}) \cdot \frac{\cot(B_{t}, C_{t})}{b_{t}}$$

$$= \frac{\cot(G_{t}, C_{t})}{\cot(S, C_{t})} \cdot \frac{\cot(B_{t}, C_{t})}{b_{t}}$$

$$\leq \frac{\cot(G_{t}, C_{t})}{k - t}.$$

► Conclude that

$$\mathbb{E}[\Phi_k] \leq \mathbb{E}[\mathsf{cost}(G_k, C_k)] \cdot (1 + 1/2 + 1/3 + \cdots + 1/k).$$

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Overall approximation bound

Use fact that $\mathbb{E}[\cos(G_k, C_k)] \leq 8 \cos(S, C^*)$ to conclude:

$$\mathbb{E}[\cos(S, C_k)] = \mathbb{E}[\cos(G_k, C_k) + \Phi_k]$$

$$\leq 8 \cos(S, C^*) \cdot (1 + H_k),$$

where $H_k = 1 + 1/2 + 1/3 + \cdots + 1/k$ is the k-th harmonic sum. \square

Bi-criteria approximation

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Bi-criteria guarantees for D^2 sampling

- ▶ Let C^* be optimal set of k centers for S.
- ▶ Algorithm provides (α, β) -approximation if it returns \widehat{C} with

$$|\widehat{C}| \leq \alpha \cdot k$$
, $\operatorname{cost}(S, \widehat{C}) \leq \beta \cdot \operatorname{cost}(S, C^*)$.

- Akin to proper $(\alpha = 1)$ and improper $(\alpha > 1)$ learning.
- ▶ D^2 sampling provides (proper) $(1, O(\log k))$ -approximation.

 - ▶ Also provides (O(1), O(1))-approximation! ▶ Tight analysis: $(O(1/\varepsilon^2), 2 + \varepsilon)$ -approximation (Wei, 2016).

Simple bi-criteria analysis

▶ Define "good" and "bad" points:

$$\mathsf{good}\colon\;\; G_t\; := \bigcup_{\substack{i \in \{1,2,\ldots,k\}:\\ \mathsf{cost}(A_i,C_t) \leq 16 \, \mathsf{cost}(A_i,\{\mu_i\})}} A_i \,,$$

$$\mathsf{bad}\colon\;\; B_t\; := \bigcup_{\substack{i \in \{1,2,\ldots,k\}:\\ \mathsf{cost}(A_i,C_t) > 16 \, \mathsf{cost}(A_i,\{\mu_i\})}} A_i \,.$$

▶ Claim. At least one of the following is true:

$$cost(S, C_t) \leq 32 cost(S, C^*),$$

 $p_t(B_t) \geq \frac{1}{2}.$

▶ **Proof**. If $cost(S, C_t) > 32 cost(S, C^*)$, then

$$p_t(B_t) = 1 - \frac{\cot(G_t, C_t)}{\cot(S, C_t)} \geq 1 - \frac{16 \cot(G_t, C^*)}{32 \cot(S, C^*)} \geq \frac{1}{2}. \quad \Box$$

Simple bi-criteria analysis (continued)

- Say round t is a "success" if
 - either $cost(S, C_{t-1}) \leq 32 cost(S, C^*)$ already,
 - or $\boldsymbol{Y}_t \in A_i \subseteq B_{t-1}$ for some cluster i, and

$$cost(A_i, C_t) \leq 16 cost(A_i, C^*)$$
 (i.e., $A_i \subseteq G_t$).

- ▶ **Claim**. Round *t* succeeds with probability 1/4 (given C_{t-1}).
- Proof.
 - ▶ If first success criterion does not hold, then

$$p_{t-1}(B_{t-1}) \geq \frac{1}{2}.$$

Furthermore, by Markov's inequality and cost bound,

$$\mathbb{P}\big(\operatorname{cost}(A_i, C_t) \leq 16\operatorname{cost}(A_i, C^*) \mid \{\boldsymbol{Y}_t \in A_i\}, C_{t-1}\big) \geq \frac{1}{2}. \quad \Box$$

▶ k success rounds guarantee $cost(S, C_t) \leq 32 cost(S, C^*)$; this happens within $t \leq 8k$ rounds with probability $1 - e^{-\Omega(k)}$.

Final remarks

- ▶ Can post-process the 8k centers by solving LP to get proper O(1)-approximation (Aggarwal, Deshpande, Kannan, 2009).
- ▶ Different local search gets proper $(9 + \epsilon)$ -approximation for any constant $\epsilon > 0$ (Kanungo et al, 2003).
 - ▶ But seems to perform worse than D^2 sampling in practice.
 - ► Can this be explained?
- ▶ Nearly all reasonable methods with theoretical analysis only pick centers from among data, thereby losing factor two in approximation. Can this be avoided?