### Coresets for Clustering Problems

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Coresets for Clustering Problems

## Basics of Coresets

- Small, weighted summary of the input.
- Given an unweighted (possibly weighted) dataset and some computational problem on this dataset, compute a small summary such that the summary approximates the dataset well for that task.

# k-means Clustering Problem

- Input: Dataset  $X \subseteq \mathbb{R}^d$ , and integer k.
- Cost function: For  $C \subseteq \mathbb{R}^d$ , |C| = k,  $\Phi(X, C) = \sum_{x \in X} \min_{c \in C} ||x - c||^2$ .

• Objective: Find set  $C \subseteq \mathbb{R}^d$  of k centers that minimizes  $\Phi(X, C)$ .

### • Coresets to *approximate the dataset well* for *k*-means.



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- Coresets to *approximate the dataset well* for *k*-means.
- How to guarantee coresets approximate dataset well.
- Coresets approximate dataset with respect to *k*-means objective function.



- Approximates the objective function for input dataset simultaneously for all queries.
- Query for *k*-means: Cost of *k*-means objective function with respect to set of *k* centers.



Coresets for Clustering Problems

## Basics of Coreset

- Let X be a dataset with non-negative weights  $\mu_X(x)$ .
- Let  $\mathcal{Q}$  be set of possible queries or solutions.
- Weighted set S is an  $\varepsilon$ -coreset of X if for all  $Q \in Q$ ,

$$(1 - \varepsilon) \mathsf{cost}(X, Q) \le \mathsf{cost}(S, Q) \le (1 + \varepsilon) \mathsf{cost}(X, Q)$$

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### $(k, \varepsilon)$ -Coreset for k-means

[HPM2004] Given a point set X ⊆ ℝ<sup>d</sup>, a weighted subset S ⊆ X is a (k, ε)-coreset of X for k-means if for all C ⊆ ℝ<sup>d</sup> such that |C| = k,

$$(1 - \varepsilon) \mathrm{cost}(X, C) \leq \mathrm{cost}(S, C, w) \leq (1 + \varepsilon) \mathrm{cost}(X, C)$$

$$\operatorname{cost}(X,C) = \sum_{x \in X} d(x,C)^2$$
,  $\operatorname{cost}(S,C,w) = \sum_{x \in S} w(x) d(x,C)^2$ .

## Basics of Coresets

- Strong coreset: If above inequality is true for all queries  $Q \in Q$ .
- Weak coreset: If above inequality is true for optimal solution  $Q^* \in \mathcal{Q}$ .

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### Basics of Coresets

#### Obtain Approximate Solutions using Coresets

- Construct coreset and solve problem on the coreset.
- Exact or approximate solution on the coreset gives approximate solution for dataset.
- We show:  $cost(X, Q_S^*) \le (1 + 2\varepsilon)cost(X, Q_X^*)$ .
- $\operatorname{cost}(X, Q_S^*) \leq \frac{1}{1-\varepsilon} \operatorname{cost}(S, Q_S^*) \leq \frac{1}{1-\varepsilon} \operatorname{cost}(S, Q_X^*) \leq \frac{1+\varepsilon}{1-\varepsilon} \operatorname{cost}(X, Q_X^*) \leq (1+2\varepsilon) \operatorname{cost}(X, Q_X^*).$

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### Applications of Coresets

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## Properties of Coresets

#### Union of Coresets is a Coreset

Let S<sub>1</sub>, S<sub>2</sub> be (k, ε)-coresets for disjoint sets X<sub>1</sub> and X<sub>2</sub>, then S<sub>1</sub> ∪ S<sub>2</sub> is a (k, ε)-coreset for X<sub>1</sub> ∪ X<sub>2</sub>.

### **Composable Coresets**

• If  $S_1$  is a  $(k, \varepsilon)$ -coreset for  $S_2$ , and  $S_2$  is a  $(k, \delta)$ -coreset for  $S_3$ , then  $S_1$  is  $(k, \varepsilon + \delta + \varepsilon \delta)$ -coreset for  $S_3$ .

• 
$$\forall C$$
,  $(1-\varepsilon) \operatorname{cost}(S_2, C, w_2) \leq \operatorname{cost}(S_1, C, w_1) \leq (1+\varepsilon) \operatorname{cost}(S_2, C, w_2)$ .

•  $\forall C$ ,  $(1-\delta)$ cost $(S_3, C, w_3) \leq$ cost $(S_2, C, w_2) \leq (1+\delta)$ cost $(S_3, C, w_3)$ .

#### Informally

If S<sub>1</sub> is coreset of S<sub>2</sub> with (1 + ε)-guarantee, and S<sub>2</sub> is coreset of S<sub>3</sub> with (1 + δ)-guarantee, then S<sub>1</sub> gives (1 + ε)(1 + δ)-guarantee for S<sub>3</sub>.

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# Merge and Reduce

• Design streaming algorithm on insertion only data streams [BS1980, HPM2004].



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# Merge and Reduce

### Storage

• log *n* levels in the tree, each level has at most one coreset:  $|S| \log n$ .

### Error of Approximation

- We compute coresets of coresets, the error of approximation goes up.
- Composing  $(k, \varepsilon)$  and  $(k, \delta)$ -coresets gives guarantee  $(1 + \varepsilon)(1 + \delta)$ .
- Guarantee using log *n* levels becomes  $(1 + \varepsilon)^{\log n}$ .

• We set 
$$\varepsilon' = \frac{\varepsilon}{\log n}$$
.

# Distributed Algorithms using Coresets

- Data partitioned across machines, they compute coreset on local data.
- Machines send coresets to the central server.
- Server computes union of coresets, coresets of coresets.
- Complexity: Communication from machine to server: Coreset size.

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### Techniques for Coreset Constructions

Coresets for Clustering Problems

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# Coresets using Uniform Sampling

- Idea: Subset of points sampled uniformly gives a coreset.
- Question: How many samples do we need? Size of coreset using uniform sampling?
- $\Omega(n)$  uniform samples.



k = 1

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# Har-Peled and Majumder (HPM2004)

- Coresets for k-means and k-median in low dimensions.
- Computes coresets of size  $O(k\varepsilon^{-d} \log n)$ .
- Let C be constant factor approximation for k-means or k-median.
- Build exponential grid of  $O(\log n)$  levels around each center.
- Snap input points to the closest point in the grid.
- Price of snapping smaller than  $\varepsilon$ OPT.
- The weighted set S is a coreset.

# Har-Peled and Kushal (2005)

- Computes coreset of size independent of *n* of size  $O(\frac{k^2}{\varepsilon^d})$  for *k*-median and  $O(\frac{k^3}{\varepsilon^{d+1}})$  for *k*-means.
- Let C be a constant factor approximation.
- Draw  $O(\frac{1}{e^{d-1}})$  lines from each center.
- Project each input point to the closest line.
- Coreset size of  $O(\frac{k}{\varepsilon})$  and  $O(\frac{k^2}{\varepsilon^2})$  for points on 1-D for k-median and k-means respectively.

# Chen's Construction (2009)

- Coreset size for k-median and k-means  $O(dk^2 \log n\varepsilon^{-2})$ .
- Key idea: Partition dataset into disjoint subsets and take random samples from each subset.
- Start with an  $(\alpha, \beta)$ -bicriteria approximation for k-means.
- Partition space using concentric rings around these centers.
- Take random samples from each ring.
- Coreset size for k-median and k-means  $O(dk^2 \log n\varepsilon^{-2})$ .

# Feldman-Langberg (2011)

- Coreset size for k-means  $\tilde{O}(k^3\varepsilon^{-4})$ .
- Samples points based on how important the points are with respect to the objective function.
- First computes sensitivity of points, and then samples points with probability proportional to sensivity.

# **Coreset Constructions**

### Coresets for k-means

Coreset Size
$O(k\varepsilon^{-d}\log n)$
$O(k^3 \varepsilon^{-(d+1)})$
$ ilde{O}(dk^2 \varepsilon^{-2} \log n)$
$ ilde{O}(dkarepsilon^{-4})$
$\tilde{O}(k^3 \varepsilon^{-4})$

### Coreset Constructions using Dimensionality Reduction

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# Coresets for k-means/k-median

Can you design coresets whose size is indepedent of d and n?
Coreset size is polynomial in k and <sup>1</sup>/<sub>c</sub>.

# Coresets for *k*-means (FSS2013)

- Assume that the data is very high dimensional.
- They give a dimensionality reduction scheme to show that most of data lies in a much smaller dimensional subspace.
- Apply known coreset constructions on data in smaller dimensional subspace.

# Coresets for *k*-means (FSS2013)

- Key idea: Cost of clustering of high dimensional points has a pseudo-random part and a structured part.
- Pseudo-random part of cost is same for all queries (with k centers).
- Structured part of the cost comes from clustering projected points.



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- Identity for k-means:  $cost(X, p) = cost(X, \mu(X)) + |X|||p \mu(X)||^2$ .
- Coreset centroid  $\mu(X)$  with weight |X| and constant  $cost(X, \mu(X))$ .

# Coresets for *k*-means (FSS 2013)

### Coreset Definition

• Let A be a set of n points in  $\mathbb{R}^d$ . A weighted set  $S \in \mathbb{R}^{m \times d}$  and a constant  $\Delta > 0$  is an  $\varepsilon$ -coreset for k-means if for all C

$$(1 - \varepsilon) cost(A, C) \leq cost(S, C) + \Delta \leq (1 + \varepsilon) cost(A, C)$$

# Coreset Construction for k-means (FSS2013)

#### Dimensionality Reduction Algorithm

- Let OPT is known for k-means.
- Compute *k*-dim subspace *S* that minimizes the sum of squared distances from points to the subspace.
- While there exists k dimensions such that adding those to S reduces the subspace approximation cost by at least  $\varepsilon^2$ OPT, add them to subspace S.
- Dimension of S is at most  $\frac{k}{r^2}$ .
- Coreset for *k*-means: Projected points on *S* (Structured part) and cost of projection onto *S* (Pseudo-random part).

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## Analysis

- Let T be the subspace containing S and C (query with k centers).
- $\operatorname{cost}(X, C) = \operatorname{cost}(X, T) + \operatorname{cost}(X_T, C) \approx \operatorname{cost}(X, S) + \operatorname{cost}(X_S, C).$
- We have  $cost(X, S) cost(X, T) \le \varepsilon^2 OPT$ .
- On avarage projected points on *T* and *S* are close. Because, cost(X<sub>T</sub>, X<sub>S</sub>) = cost(X, S) − cost(X, T) ≤ ε<sup>2</sup>OPT.
- Show that  $|\operatorname{cost}(X_{\mathcal{S}}, C) \operatorname{cost}(X_{\mathcal{T}}, C)| \leq \varepsilon \mathsf{OPT}.$



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### FSS13

• Let A be a set of n points in  $\mathbb{R}^d$ , equivalently,  $A \in \mathbb{R}^{n \times d}$ . Let  $A_m$  be its rank *m*-approximation for  $m = O(\frac{k}{\varepsilon^2})$ . Then, there exists a constant  $\Delta = ||A - A_m||_F^2$  such that for all sets of k centers C,

$$(1-arepsilon) \mathsf{cost}(\mathsf{A},\mathsf{C}) \leq \mathsf{cost}(\mathsf{A}_m,\mathsf{C}) + \Delta \leq (1+arepsilon) \mathsf{cost}(\mathsf{A},\mathsf{C})$$

### Coreset

- We have *n* points on  $O(\frac{k}{\varepsilon^2})$ -dimensional subspace *S*, and a constant equals the projection cost on subspace *S*.
- We apply Feldman-Langberg coreset construction on S to obtain a coreset of size  $\tilde{O}(\frac{k^2}{\varepsilon^6})$ .

# Coresets for k-median Problem

### Euclidean k-median Problem

Given a set X of n points in ℝ<sup>d</sup>, and an integer k, the objective is to find a set C ⊆ ℝ<sup>d</sup> of k centers such that the objective function

$$\sum_{x\in X}\min_{c\in C}||x-c||_2$$

is minimized.

• *k*-median is NP-hard, and constant factor approximation algorithms are known for *k*-median.

- Many results on designing strong coresets for k-median.
- Feldman-Langberg framework for k-median has coreset of size  $\frac{kd}{\epsilon^2}$ .

### Focus for this talk

Woodruff-Sohler designs a coreset for k-median of size poly(k, <sup>1</sup>/<sub>ε</sub>), independent of d.

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# Coreset for *k*-median (Woodruff-Sohler'18)

- Can we get a coreset for k-median similar to k-means?
- Let X<sub>S</sub> be the set of projected points on subspace S and a constant Δ. Do we have for all queries C,

$$(1 - \varepsilon) \mathsf{cost}(X, C) \le \mathsf{cost}(X_S, C) + \Delta \le (1 + \varepsilon) \mathsf{cost}(X, C)$$

• Gave a counterexample to any such guarantee for k-median.

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# Coreset for *k*-median (Woodruff-Sohler'18)

### Counterexample for k = 1

- Let there be *n* points on a unit ball in  $\mathbb{R}^d$  for very high *d*.
- We project these points on a  $I = poly(k, \frac{1}{\varepsilon})$ -dimensional subspace.
- With high probability, norms of the projected points are very small.
- For query with center at origin, we require  $\Delta = n$ .
- For query with center at {1,0, · · · ,0}, we get cost of original points as √2n and total cost of coreset and constant is 2n.

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# Coreset for *k*-median (Woodruff-Sohler'18)

 Unlike for k-means, we cannot apply Pythagorean theorem here to split the cost among the cost of projection and cost of clustering of projected points.

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## Coreset for *k*-median (Woodruff-Sohler'18)

- Show that a variant of dimensionality reduction scheme works for *k*-median.
- Dimensionality reduction gives a set *n* points in  $\mathbb{R}^{d+1}$  such that most of the points live in a much smaller dimensional subspace.

### Coreset for *k*-median (Woodruff-Sohler'18)

• Key idea: Add a special dimension to any point with value equal to the distance to subspace *S*.

### **Dimensionality Reduction**

#### Dimensionality Reduction Algorithm

- Let Opt be the cost of the optimal k-median clustering.
- Compute optimal *k*-dimensional subspace S for minimizing sum of distances from points to subspace S.
- While we can add k dimensions to S to reduce the cost of the subspace approximation problem by  $\varepsilon^2 OPT$ , do that.
- Let S be the best such subspace.
- For each point *p* in *X*,
  - **(**) Compute distance  $d(p, p_S)$  where  $p_S$  is the projection on subspace S.

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2 Return  $(p_S, d(p, p_S)) \in \mathbb{R}^{d+1}$ 

### Analysis

- Let T denote the subspace containing both S and C.
- For any center  $c_p \in C$ , we have  $d(p, c_p) = (d(p, p_T)^2 + d(p_T, c_p)^2)^{1/2}$ .
- Cost with respect to the coreset is  $d((p_5, d(p, p_5), (c_p, 0)) = (d(p_5, c_p)^2 + d(p, p_5)^2)^{1/2}.$
- (Distance to Subspace Lemma)  $cost(X, S) - cost(X, T) = \sum_{p} (d(p, p_{S}) - d(p, p_{T})) \le \varepsilon^{2} OPT.$
- (Distance inside Subspace Lemma)  $\sum_{p \in X} |d(p_T, c_p) - d(p_S, c_p)| \le \varepsilon \text{OPT}.$

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### Distance inside Subspace Lemma

• To show: 
$$\sum_{p \in P} |d(p_T, c_p) - d(p_S, c_p)| \le \varepsilon \text{OPT}.$$

- Using triangle inequality, this is at most  $cost(X_S, X_T)$ .
- For all  $p \in Q$  such that  $d(p_T, p_S) \le \varepsilon d(p, p_S)$ , we have  $\sum_{p \in Q} d(p_T, p_S) \le \varepsilon OPT$ .
- Else,  $d(p_T, p_S) = (d(p, p_S)^2 d(p, p_T)^2)^{1/2}$ .
- Since d(p<sub>T</sub>, p<sub>S</sub>) > εd(p, p<sub>S</sub>), using triangle inequality, we have above expression is at most <sup>d(p,p<sub>S</sub>)-d(p,p<sub>T</sub>)</sup>/<sub>ε</sub>.
- Since  $\sum_{p} d(p, p_{S}) d(p, p_{T}) \leq \varepsilon^{2} \text{OPT}$ , we are done.

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### Analysis contd.

• 
$$|\operatorname{cost}(S,C) - \operatorname{cost}(X,C)| \le \varepsilon \operatorname{cost}(X,C).$$

• We show:  $\sum_p |d(p,c_p) - d((p_S,d(p,p_S),(c_p,0))| \le 2\varepsilon \text{OPT}.$ 

$$\begin{aligned} |d(p, c_p) - d((p_S, d(p, p_S), (c_p, 0))| \\ &= |(d(p, p_T)^2 + d(p_T, c_p)^2)^{1/2} - (d(p, p_S)^2 + d(p_S, c_p)^2)^{1/2}| \\ &= |d(p, p_T), d(p_T, c_p)|_2 - |d(p, p_S), d(p_S, c_p)|_2 \\ &\leq |d(p, p_T) - d(p, p_S), d(p_T, c_p) - d(p_S, c_p)|_2 \\ &\leq |d(p, p_T) - d(p, p_S), d(p_T, c_p) - d(p_S, c_p)|_1 \\ &= |d(p, p_T) - d(p, p_S)| + |d(p_T, c_p) - d(p_S, c_p)| \\ &\leq 2\varepsilon \mathsf{OPT} \end{aligned}$$

using Distance to Subspace Lemma and Distance inside Subspace Lemma

### Thanks & Questions

Coresets for Clustering Problems

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# Sampling-based Algorithms for Clustering Problems

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Sampling-based Algorithms for Clustering Problems

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Sampling-based Algorithms for Clustering Problems

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k-means Clustering

### k-means Clustering Problem

- Input: Dataset  $X \subseteq \mathbb{R}^d$ , and integer k.
- Cost function: For  $C \subseteq \mathbb{R}^d$ , |C| = k,  $\Phi(X, C) = \sum_{x \in X} \min_{c \in C} ||x - c||^2$ .

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Sampling-based Algorithms for Clustering Problems

- Input: Dataset  $X \subseteq \mathbb{R}^d$ , and integer k.
- Cost function: For  $C \subseteq \mathbb{R}^d$ , |C| = k,  $\Phi(X, C) = \sum_{x \in X} \min_{c \in C} ||x - c||^2$ .



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Objective: Find set C ⊆ ℝ<sup>d</sup> of k centers that minimizes Φ(X, C).

- Input: Dataset  $X \subseteq \mathbb{R}^d$ , and integer k.
- Cost function: For  $C \subseteq \mathbb{R}^d$ , |C| = k,  $\Phi(X, C) = \sum_{x \in X} \min_{c \in C} ||x - c||^2$ .
- Objective: Find set C ⊆ ℝ<sup>d</sup> of k centers that minimizes Φ(X, C).



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- Input: Dataset  $X \subseteq \mathbb{R}^d$ , and integer k.
- Cost function: For  $C \subseteq \mathbb{R}^d$ , |C| = k,  $\Phi(X, C) = \sum_{x \in X} \min_{c \in C} ||x - c||^2$ .
- Objective: Find set C ⊆ ℝ<sup>d</sup> of k centers that minimizes Φ(X, C).
- Voronoi partitioning gives k clusters.



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# Known Results: k-means Clustering

•  $\alpha$ -approximation ALG: for any instance *I*, ALG(*I*)  $\leq \alpha \cdot OPT(I)$ .

Hardness Results

Approximation Algorithms

NP-hard for  $k \ge 2$  [D2008]6.357 by Ahmadian *et al.* (2016)NP-hard for  $d \ge 2$  [V2009,MNV2012] $(1 + \varepsilon)$  in  $O(nd2^{\tilde{O}(\frac{k}{\varepsilon})})$  [JKS2014]APX-hard [Awasthi *et al.* (2015)]

Sampling-based Algorithms for Clustering Problems

### Approximation Algorithm for k-means

Sampling-based Algorithms for Clustering Problems

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• Objective function:  $\min_{c \in \mathbb{R}^d} \Phi(X, \{c\}) = \min_{c \in \mathbb{R}^d} \sum_{x \in X} ||x - c||^2$ .

### Exact Solution

• Centroid of points is the optimal center for 1-means.

#### Approximate Solution

• A uniformly sampled point gives 2-approximation in expectation.

• Fact: 
$$\Phi(X, p) = \Phi(X, \mu(X)) + |X| \cdot ||p - \mu(X)||^2$$

 Centroid of O(<sup>1</sup>/<sub>ε</sub>) points sampled uniformly at random gives (1+ε)-approximation for 1-means with constant probability [IKI1994].

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• 2-means is NP-hard.

### Approximate Solution

 Require a sample of size O(<sup>1</sup>/<sub>ε</sub>) chosen uniformly at random from each of the optimal clusters.

#### Approximate Solution

Require a sample of size O(<sup>1</sup>/<sub>ε</sub>) chosen uniformly at random from each of the optimal clusters.

#### Approximate Larger Optimal Cluster

- Uniformly sample <sup>2</sup>/<sub>ε</sub> points. Sample contains at least <sup>1</sup>/<sub>ε</sub> points from the larger optimal cluster.
- Consider all subsets of size  $\frac{1}{\varepsilon}$  of the sample. Running time  $\left(\frac{\frac{2}{\varepsilon}}{1}\right)$ .
- Centroid of these subsets are candidate centers for the optimal center of the larger cluster.

#### Approximate Smaller Optimal Cluster

• How do you approximate the center for the smaller optimal cluster?

#### Approximate Smaller Optimal Cluster

• How do you approximate the center for the smaller optimal cluster?

#### Prune and Sample

- For each of the candidate centers of the larger optimal cluster, consider the set Q of farthest <sup>n</sup>/<sub>2i-1</sub> points from the candidate center for 1 ≤ i ≤ log n.
- Randomly sample O(<sup>1</sup>/<sub>ε<sup>2</sup></sub>) points from Q. Consider all possible subsets of size O(<sup>1</sup>/<sub>ε</sub>) from the sample.
- Centroid of at least one subset gives  $(1 + \varepsilon)$ -approximation for the smaller optimal cluster.
- Same idea works for any  $k \ge 2$  [KSS2010].

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# Sampling based $(1 + \varepsilon)$ -approximations for k-means

#### Approximate Largest Optimal Cluster

- Step 1: Uniformly sample  $O(\frac{k}{\epsilon})$  points.
- Whp, sample contains O(<sup>1</sup>/<sub>ε</sub>) points from largest optimal cluster.
- Step 2: Consider means of subsets of size O(<sup>1</sup>/<sub>ε</sub>) of sample.
- Approximates cluster in time  $O(\frac{k}{\varepsilon})^{O(\frac{1}{\varepsilon})}$ .



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# Sampling based $(1 + \varepsilon)$ -approximations for k-means

#### Approximate Smaller Optimal Clusters

- Number of points in some optimal clusters may be very small.
- Uniform sampling does not help to approximate smaller clusters.



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# $D^2$ -Sampling

### $D^2$ -Sampling

- Let C be set of already chosen centers.
- D<sup>2</sup>-sampling chooses point p as next center wp prop. to min<sub>c∈C</sub> ||p − c||<sup>2</sup>.



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### $D^2$ -Sampling based Algorithms

- k centers using  $D^2$ -sampling gives  $O(\log k)$ -approximation [AV2007].
- O(k) such centers give constant pseudo-approximation [ADK2009].

# $D^2$ -Sampling based Algorithms

- k centers using  $D^2$ -sampling gives  $O(\log k)$ -approximation [AV2007].
- O(k) such centers give constant pseudo-approximation [ADK2009].

#### *k*-means++

- A point is sampled from an *uncovered* optimal cluster, that cluster is well-approximated.
- Overall (log k)-approximation because may miss some clusters.
- Lower bound of  $\Omega(\log k)$  for k-means++.

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# Sampling based $(1 + \varepsilon)$ -approximations for k-means

### $D^2$ -Sampling based Algorithm

- Iterative algorithm, *C<sub>i</sub>* be chosen centers till *i*th iteration.
- Step 1: S is  $D^2$ -sample with respect to  $C_i$  of  $O(\frac{k}{\varepsilon^3})$  points.
- Step 2: Consider mean of subsets of size O(<sup>1</sup>/<sub>ε</sub>) of sample.



•  $(1 + \varepsilon)$ -approx for k-means in time  $O(nd \cdot 2^{\tilde{O}(\frac{k}{\varepsilon})})$  [JKS2014].

### Constrained Clustering: Examples

- Given *n* points in  $\mathbb{R}^d$ , and integer *k*.
- Objective function:  $\sum_{x \in X} \min_{c \in C} ||x c||^2$
- Minimize objective while obeying additional constraints.
- Examples of constraints:
  - *r*-gather clustering: Each cluster has size at least *r*.
  - Capacitated clustering: Cluster sizes have upper bounds.
  - Chromatic clustering: No two points in cluster with same color.

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Figure : *r*-gather clustering: Input points in  $\mathbb{R}^2$ , k = 2, r = 20

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### Constrained Clustering: Examples

- *r*-gather clustering: Each cluster has size at least *r*.
- Unconstrained *k*-means clustering on the input instance.



Figure : Solution for Unconstrained clustering

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## Constrained Clustering: Examples

• *r*-gather clustering: Each cluster has size at least *r*.



Figure : *r*-gather clustering: Input points in  $\mathbb{R}^2$ , k = 2, r = 20

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### Constrained k-means Problem

- Constrained k-means [Ding & Xu 2015]: Given n points in ℝ<sup>d</sup>, integer k, and set of constraints, find k clusters which minimize objective function.
- $(1 + \epsilon)$ -approximation for constrained *k*-means [Ding & Xu 2015].

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### Constrained k-means Problem

- Locality property: Points in the same cluster are closer to each other.
- True for unconstrained clustering.
- Locality not valid for constrained clustering.



Figure : *r*-gather Clustering: Input points in  $\mathbb{R}^2$ , k = 2, r = 20

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# Cluster Assignment: Find Clusters from Centers

- Find clusters given k centers.
- Voronoi partitioning works for unconstrained clustering.
- Constrained clustering: [Ding & Xu 2015] Designed polynomial time assignment algorithms for various constrained *k*-means problems.

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# Cluster Assignment Algorithm

- Find clusters minimizing objective while satisfying constraints.
- Assignment algorithm for r-gather clustering [Ding & Xu 2015]
- Reduces to min-cost circulation problem.



Figure : Assignment algorithm for r-gather Clustering

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### Constrained *k*-means: Known Results

- Number of candidate centers  $L \leq O((\log n)^k 2^{\operatorname{poly}(\frac{k}{\epsilon})})$ .
- Assignment takes P(X) time to find clustering cost.
- Ding & Xu give  $(1 + \epsilon)$ -approximation in time  $O(nd \cdot L + P(X) \cdot L)$ .

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### List k-means Problem

- Given  $X \subseteq \mathbb{R}^d$ , integer  $k, \epsilon > 0$ , implicit OPT partition  $X_1, \ldots, X_k$ .
- List k-means finds a set  $C = \{C_1, \ldots, C_L\}$ .
- Each  $C_i$  is set of k centers.
- Such that  $\exists j \in [1, L]$ ,  $C_j$  gives  $(1 + \epsilon)$ -approximation wrt  $X_1, \ldots, X_k$ .

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### List *k*-means to Constrained *k*-means

- List k-means outputs a list of candidate k-centers.
- For each *k*-center, compute clustering using assignment algorithm.
- The clustering with minimum cost would be the solution for constrained *k*-means.

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### List k-means

- List size in [Ding & Xu] is  $L \leq O((\log n)^k 2^{\operatorname{poly}(\frac{k}{\epsilon})})$
- [BJK2018] has list size  $L \leq 2^{\tilde{O}(\frac{k}{\epsilon})}$
- Notice that list size is independent of *n*.
- Almost matching lower bound:  $L \ge 2^{\tilde{\Omega}(\frac{k}{\sqrt{\epsilon}})}$
- Running time:  $O(nd \cdot L + P(X) \cdot L)$

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- Almost matching lower bound:  $L \ge 2^{\tilde{\Omega}(\frac{k}{\sqrt{\epsilon}})}$
- Running time:  $O(nd \cdot L + P(X) \cdot L)$
- Can be extended for List k-median problem.

## **Constrained Clustering**

- For the largest OPT cluster things are fine.
- $D^2$ -sampling based scheme does not work for constrained clustering.



Figure :  $D^2$ -sampling points, k = 2

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## **Constrained Clustering**

• Centroid of none of the subsets may be good.



Figure :  $D^2$ -sampling points, k = 2

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# Idea: Constrained Clustering

- Cluster misses representation if portions of it close to covered clusters.
- Idea: Add  $O(\frac{1}{\epsilon})$  copies of centers in C to the set of sampled points.
- Trying all subsets of this new set works.
- We obtain  $(1 + \epsilon)$ -approximation for List k-means with  $L = 2^{\tilde{O}(\frac{k}{\epsilon})}$ .

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#### Thanks & Questions

Sampling-based Algorithms for Clustering Problems

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