One-pass approximate *k*-means optimization

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One-pass streaming setting

Streaming setting is similar to online setting, however data stream is finite.

Motivation: very large data-sets, and/or resource constraints (time, memory).

Goal: algorithms that are light-weight (time, memory), and make only one-pass over the data.

We study unsupervised learning, in the streaming setting.

Feedback is extremely limited: NO labels, but algorithm can compute intermediate values of the objective function, on points seen so far.

k-means clustering objective

Clustering algorithms can be hard to evaluate without prior information or assumptions on the data.

With no assumptions on the data, one evaluation technique is w.r.t some objective function.

A widely-cited and studied objective is k-means: Given set, $X \subset R^d$, choose $C \subset R^d$, $|C| = k$, to minimize:

$$\phi_C = \sum_{x \in X} \min_{c \in C} \|x - c\|^2$$

Optimizing k-means is NP hard, even for k=2 [DFKV '04].

Widely-used algorithm of same name [Lloyd '57]. Fast but lacks approximation guarantee, and can suffer from bad initialization.

Related work

[Arthur & Vassilvitskii, SODA '07]: *k*-means++, a batch clustering algorithm with O(log *k*)-approx. of *k*-means.

[Guha, Meyerson, Mishra, Motwani, & O'Callaghan, TKDE '03]: Divide and conquer streaming (a,b)-approximate *k*-medoid clustering.

Definition: b-approximation: $\frac{\phi_C}{\phi_{OPT}} \leq b$

Definition: Bi-criteria (a,b)-approximation guarantee: a$\cdot$*k* centers, b-approx.

Contributions

Extend *k*-means++ to k-means#, an (O(log *k*), O(1))-approximation to k-means, in batch setting.

Analyze Guha *et al.* divide and conquer algorithm, using (a,b)-approximate *k*-means clustering.

Use Guha *et al.* with k-means# and then k-means++ to yield a one-pass O(log k)-approximation algorithm to *k*-means objective.

Analyze multi-level hierarchy version for improved memory vs. approximation tradeoff.

Experiments on real and simulated data.

k-means++

Algorithm:

Choose first center c_1 uniformly at random from X, and let $C = \{c_1\}$.

Repeat (k-1) times:

Choose next center $c_i = x' \in X$ with prob. $\frac{D(x',C)^2}{\sum_{x\in\mathcal{X}} D(x,C)^2}$

$C \leftarrow C \cup \{c_i\}$

where $D(x,C) = \min_{c\in C} \|x - c\|$

Theorem (Arthur & Vassilvitskii '07): Returns an O(log *k*)-approximation, in expectation.

k-means#

Idea: *k*-means++ returns *k* centers, with O(log *k*)-approximation. Can we design a variant that returns O(*k* log *k*) centers, but constant approximation?

Algorithm:

```
Initialize C={}.

Choose 3·log(k) centers independently and uniformly
at random from X, and add them to C.

Repeat (k-1) times:

    Choose 3·log(k) centers indep. with prob.
    and add them to C.
```

$$\frac{D(x',C)^2}{\sum_{x\in\mathcal{X}} D(x,C)^2}$$

k-means#

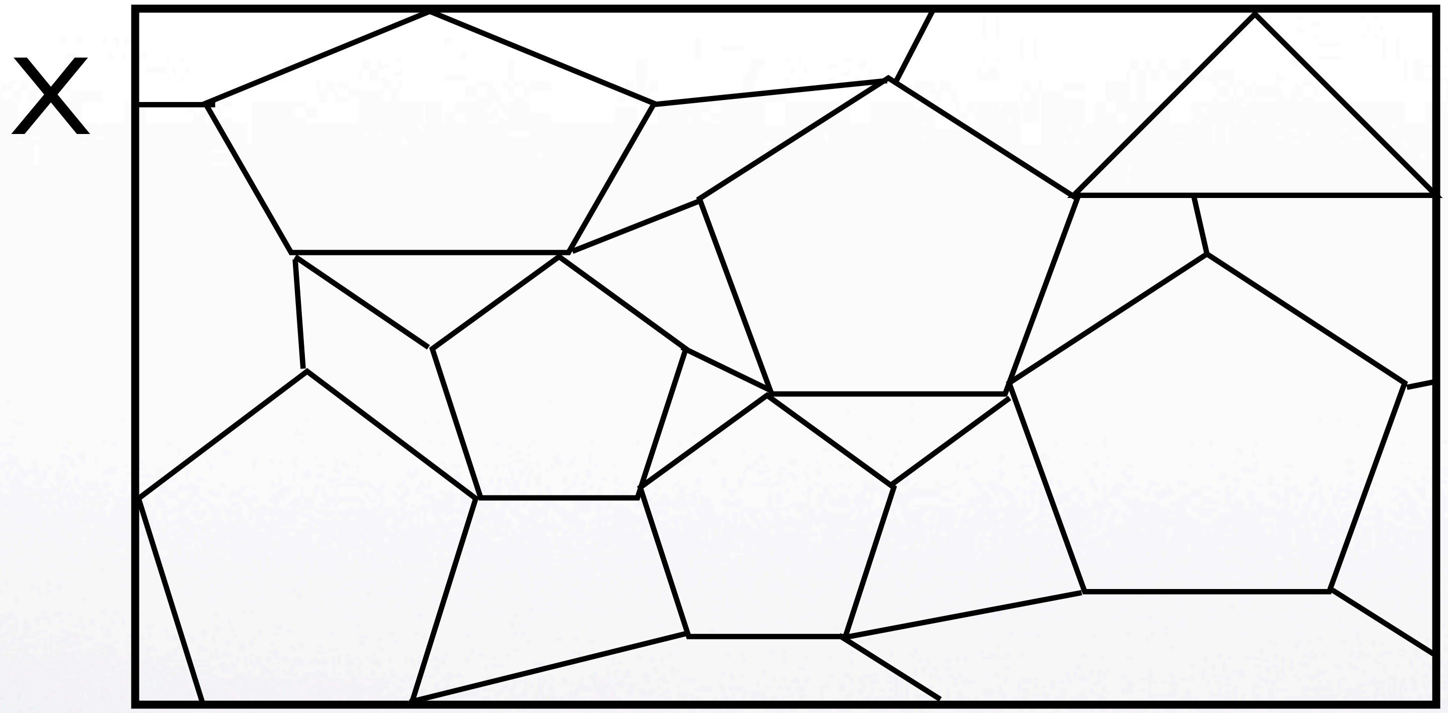
Theorem: With probability at least 1/4, *k*-means# yields an O(1)-approximation, on O(*k* log *k*) centers.

Corollary: With probability at least 1-1/n, running *k*-means# for 3·log *n* independent runs yields an O(1)-approximation (on O(*k* log *k*) centers).

Proof: Call it repeatedly, 3·log *n* times, independently, and choose the clustering that yields the minimum cost. Corollary follows, since

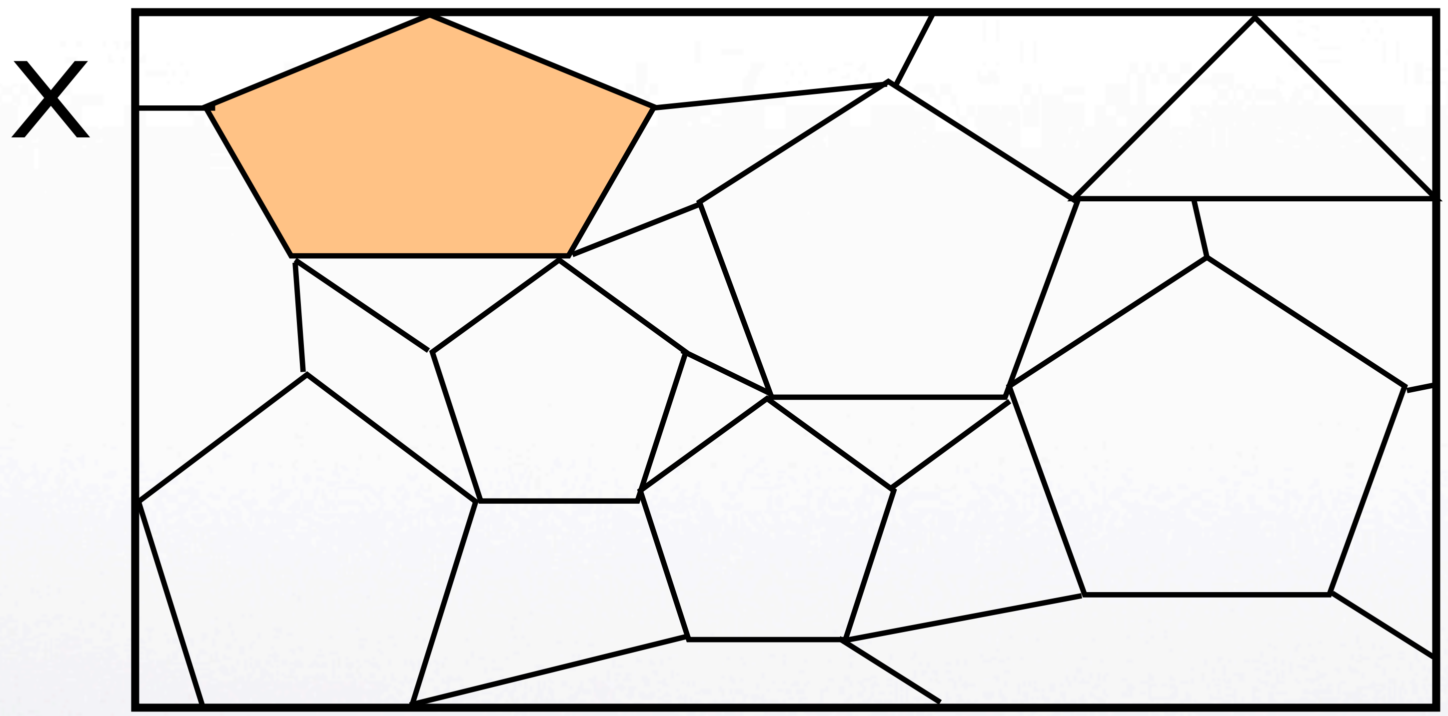
$$\left(1-(3/4)^{3\log n}\right) \geq \left(1-\frac{1}{n}\right).$$

k-means# proof idea



The clustering (partition) induced by OPT.

k-means# proof idea



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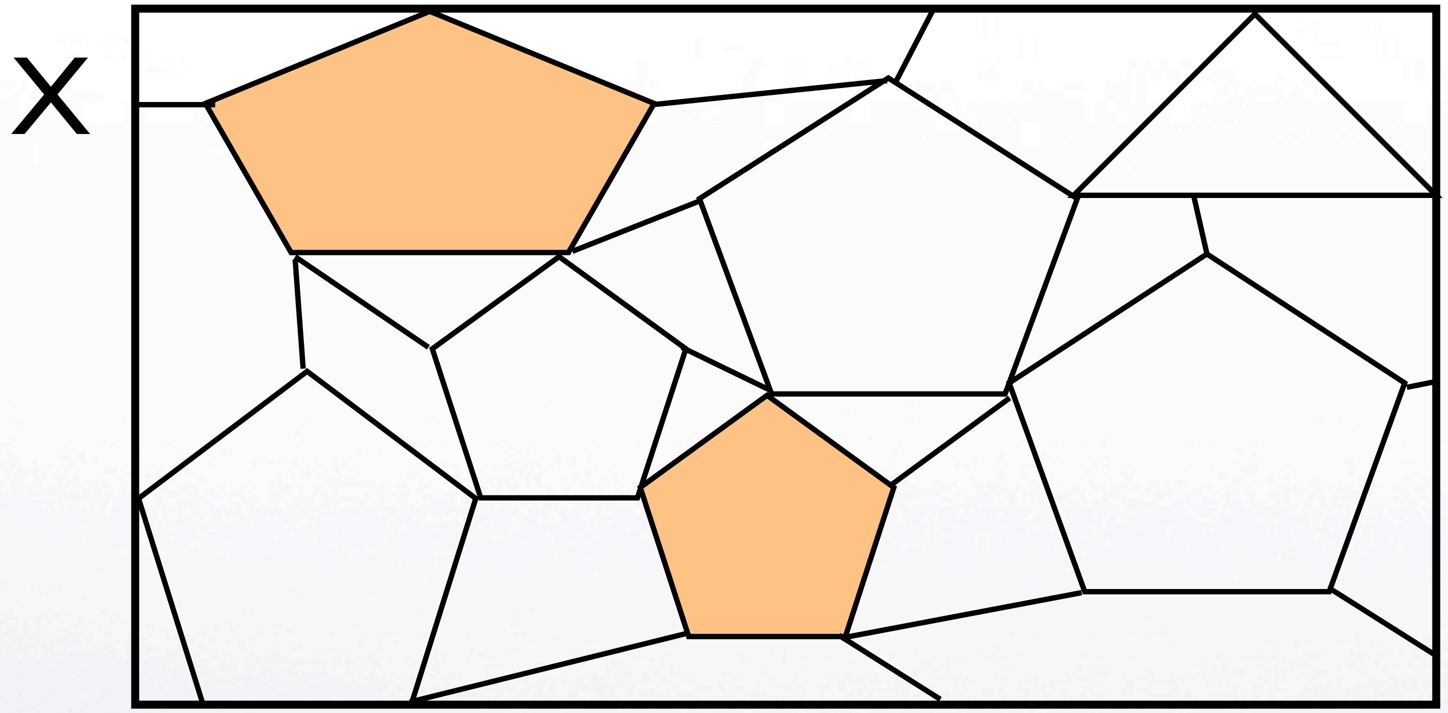

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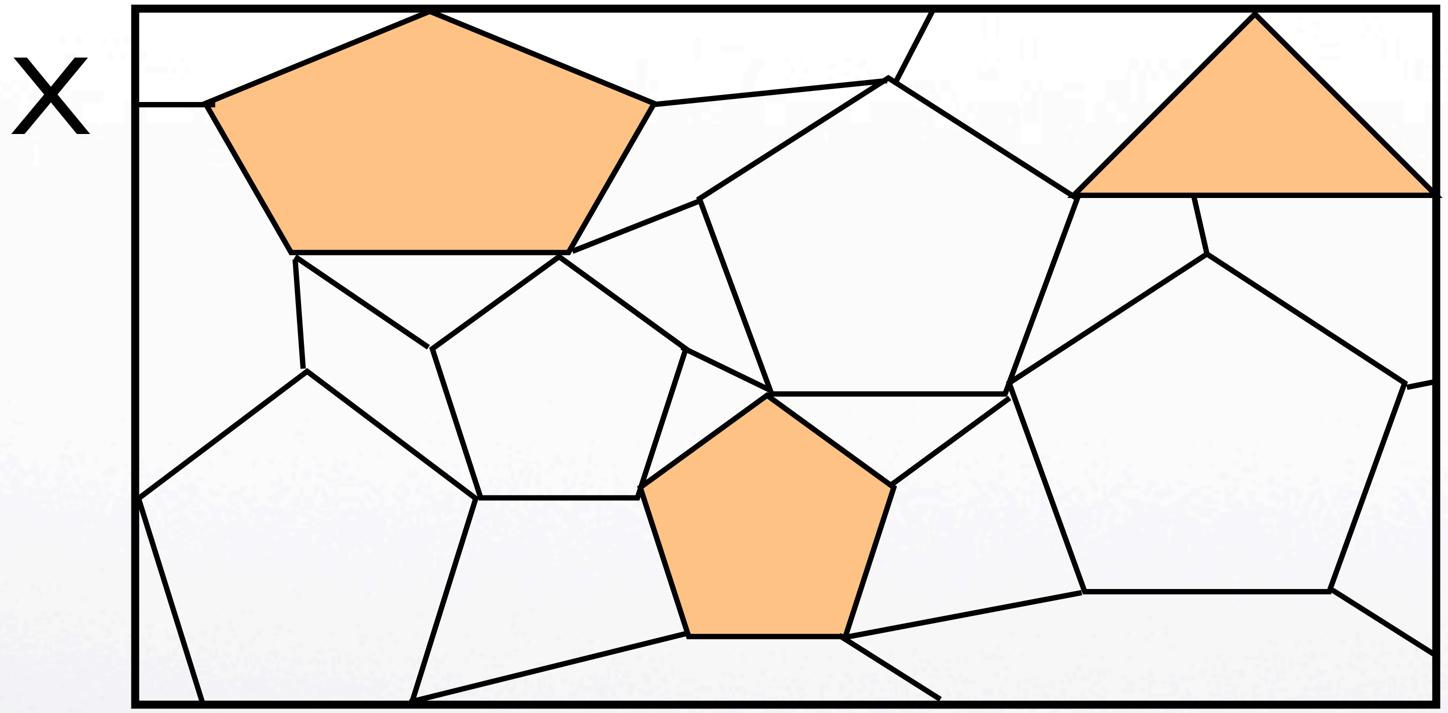
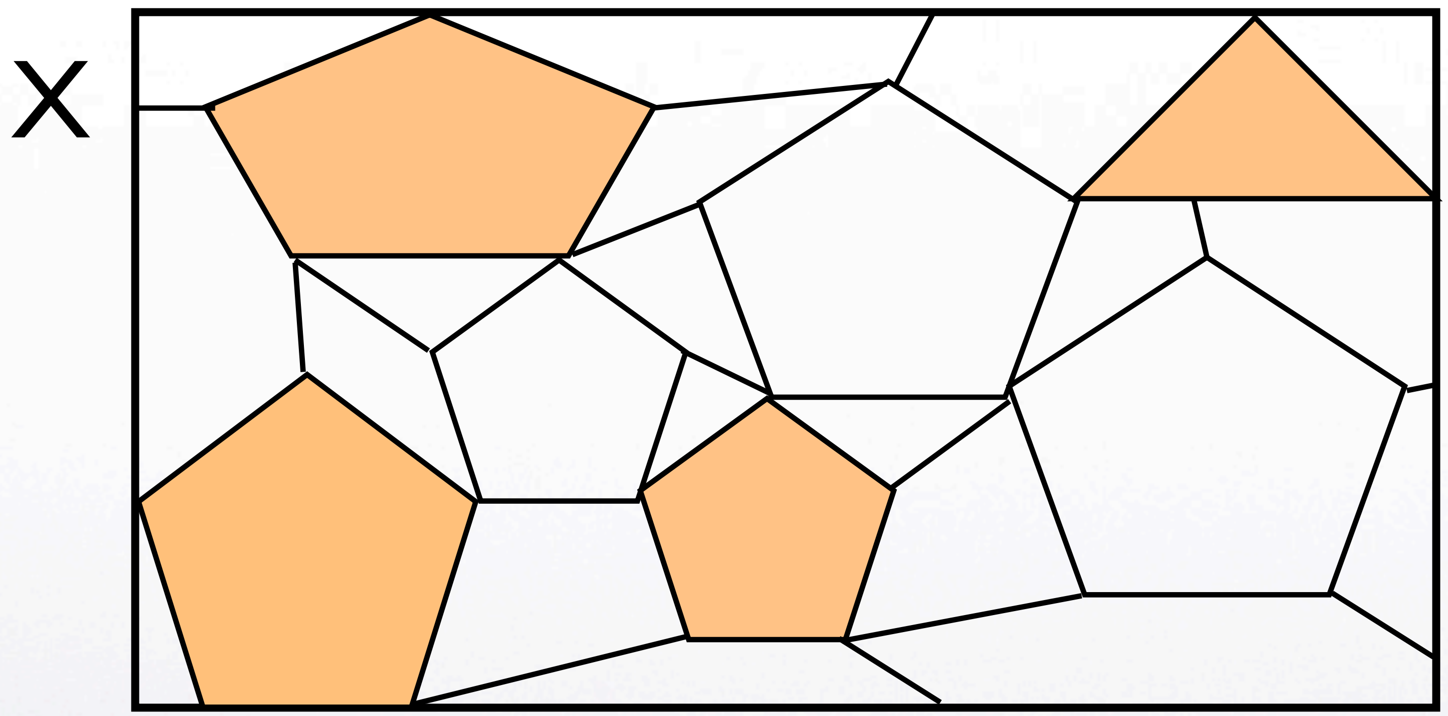
k-means# proof idea



The clustering (partition) induced by OPT.

k-means# proof idea



The clustering (partition) induced by OPT.

→ We cover the *k* clusters in OPT, after choosing O(*k* log *k*) centers.

k-means#

Theorem: With probability at least 1/4, *k*-means# yields an O(1)-approximation, on O(*k* log *k*) centers.

Proof outline: Definition "covered": cluster A ∈ OPT is covered if: $\phi_C(A) < 32 \cdot \phi_{OPT}(A)$, where $\phi_C(A) = \sum_{x \in A} D(x, C)^2$.

Define $\{X_c, X_u\}$: the partition of X into covered, uncovered.

In the first round we cover one cluster in OPT. In any later round, either:

Case 1: $\phi_C(X_c) > \phi_C(X_u)$: We are done.

Case 2 : $\phi_C(X_c) \le \phi_C(X_u)$: We are likely to cover another OPT cluster.

k-means# proof

Fix any point x chosen in the first step. Define A as the unique cluster in OPT, s.t. x $\in$ A.

Lemma (AV '07): Fix A $\in$ OPT, and let C be the 1-clustering with the center chosen uniformly at random from A. Then $E[\phi_C(A)] = 2 \cdot \phi_{OPT}(A)$.

Corollary: $Pr[\phi_C(A) < 8 \cdot \phi_{OPT}(A)] \geq 3/4$. Pf. Apply Markov's inequality.

After $3 \cdot \log(k)$ random points, probability of hitting a cluster A with a point that is good for A is at least (1-1/k).

So after first step, w.p. at least (1-1/k), at least 1 cluster is covered.

k-means# proof

Case 1: $\phi_C(X_c) > \phi_C(X_u)$.

Since X= $X_c \cup X_u$ and by definition of ϕ,

$$\phi_C(X) = \phi_C(X_c) + \phi_C(X_u) \leq 2 \cdot \phi_C(X_c) \leq 64 \cdot \phi_{OPT}(X_c) \leq 64 \cdot \phi_{OPT}(X)$$

by definition of Case 1, and definition of covered.

Last inequality is by $X_c \subseteq X$, and definition of ϕ.

k-means# proof

Case 2: $\phi_C(X_c) \leq \phi_C(X_u)$.

The probability of picking a point in X_u at the next round is:

$$\frac{\sum_{x \in X_u} D(x,C)^2}{\sum_{x \in X} D(x,C)^2} = \frac{\phi_C(X_u)}{\phi_C(X_u) + \phi_C(X_c)} \geq \frac{1}{2}$$

Lemma (AV '07): Fix A ∈ OPT, and let C be any clustering. If we add a center to C, sampled randomly from the D^2 weighting over A, yielding C' then: $E[\phi_{C'}(A)] \leq 8 \cdot \phi_{OPT}(A)$. Corollary: $Pr[\phi_{C'}(A) < 32 \cdot \phi_{OPT}(A)] \geq 3/4$

So, w.p. $\geq \frac{1}{2} \cdot \frac{3}{4} = \frac{3}{8}$ we pick a point in X_u that covers a new cluster in OPT

So after 3·log(*k*) picks, prob. of covering a new cluster is at least (1-1/k).

k-means# proof summary

For the first round, prob. of covering a cluster in OPT is at least (1-1/k).

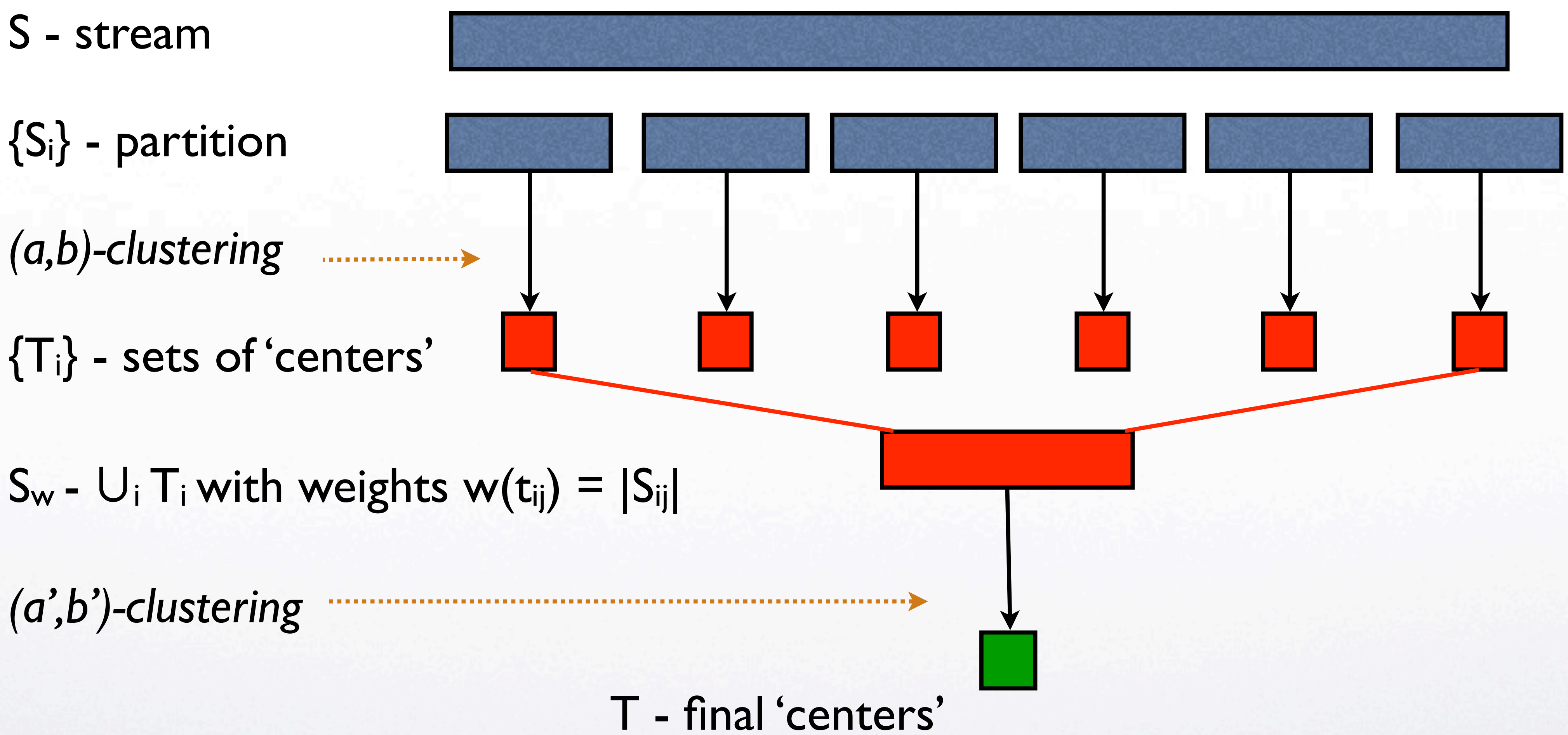
For the k-1 remaining rounds, either Case 1 holds, and we have achieved a 64-approximation, or Case 2 holds, and the probability of covering a new cluster in OPT, in the next round, is at least (1-1/k).

So the probability that after *k* rounds there exists an uncovered cluster in OPT is $\leq 1-(1-1/k)^k \leq 3/4$.

Thus the algorithm achieves a 64-approximation on $3k \cdot \log(k)$ centers, with probability at least 1/4.

Corollary: Repeating it $3 \cdot \log(n)$ times yields probability (1-1/n).

Divide and conquer clustering



[Guha *et al.* '03] analyzed for *k*-medoid clustering: (a', O(bb'))-approximation.

One-pass *k*-means approx.

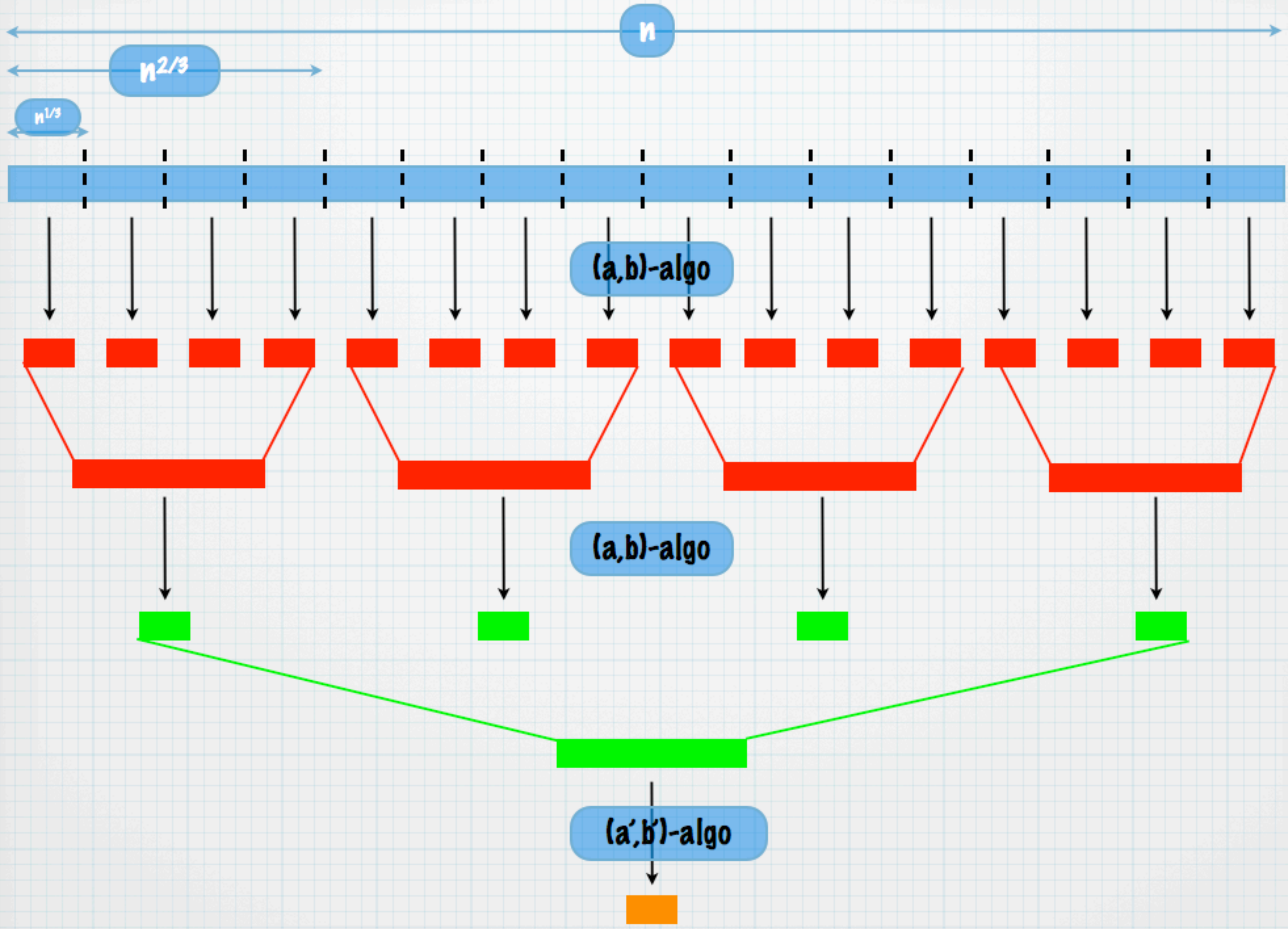
We first analyze Guha *et al.* scheme for (a,b)-approximation algorithms w.r.t. *k*-means: yields a one-pass (a’,O(bb’))-approximation algorithm.

Our algorithm:

For the (a,b) algorithm, use (repeated) k-means#: a = O(log *k*), b = O(1).

For the (a’,b’) algorithm, use k-means++: a’= 1, b’ = O(log k)

So the combined algorithm is a (1, O(log k))-approximation to *k*-means.



n
n^{2/3}
n^{1/3}
(a,b)-algo
(a,b)-algo
(a',b')-algo

Memory vs. approximation

Generalize to multi-level hierarchy; idea in Guha *et al.*

Call repeated k-means# at all levels but the last, and k-means++ at the last.

Theorem: Given memory $M = n^{\alpha}$ for a fixed $\alpha > 0$, letting $r = 1/\alpha$ yields an r-level one-pass algorithm with $O(c^{r-1} \log k)$-approximation.

Note: Unit of memory is a word; a point in R^d can be stored in $O(1)$ space.

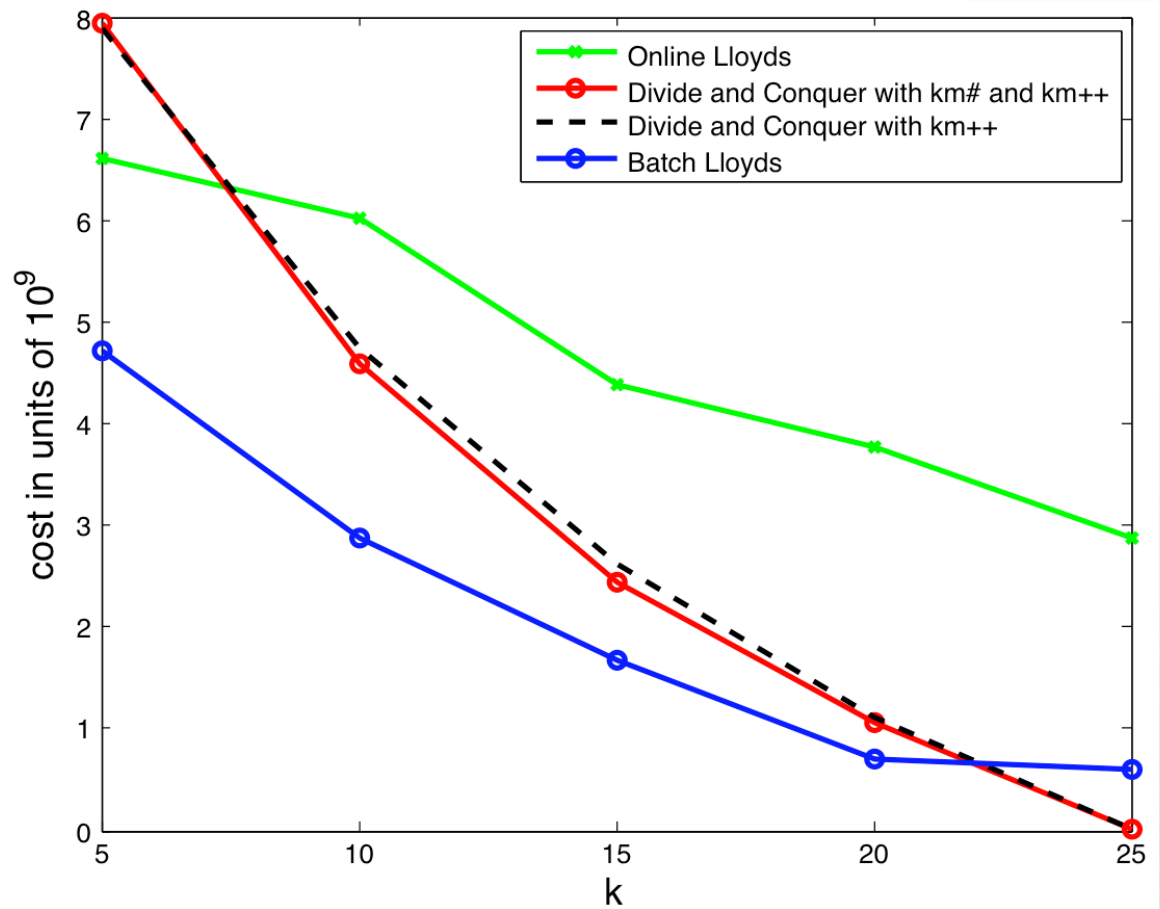
Experiments

k	BL	OL	DC-1	DC-2	BL	OL	DC-1	DC-2
5	$4.7254 \cdot 10^9$	$6.5967 \cdot 10^9$	$7.9336 \cdot 109$	$7.8752 \cdot 109$	5.80	1.44	16.95	12.22
10	$2.8738 \cdot 10^9$	$6.0146 \cdot 10^9$	$4.5968 \cdot 10^9$	$4.7288 \cdot 10^9$	7.33	2.76	53.10	24.74
15	$1.6753 \cdot 10^9$	$4.3743 \cdot 10^9$	$2.4338 \cdot 10^9$	$2.6280 \cdot 10^9$	8.85	4.00	112.68	36.86
20	$7.0016 \cdot 10^8$	$3.7794 \cdot 10^9$	$1.0661 \cdot 10^9$	$1.1017 \cdot 10^9$	11.75	6.04	250.21	48.57
25	$6.0011 \cdot 10^8$	$2.8859 \cdot 10^9$	$2.7493 \cdot 10^5$	$2.7906 \cdot 10^5$	13.83	7.00	403.81	60.96

Table 1: norm25 dataset. (columns 2-5 has the clustering cost and columns 6-9 has time in sec.)

Mixture of 25 Gaussians:

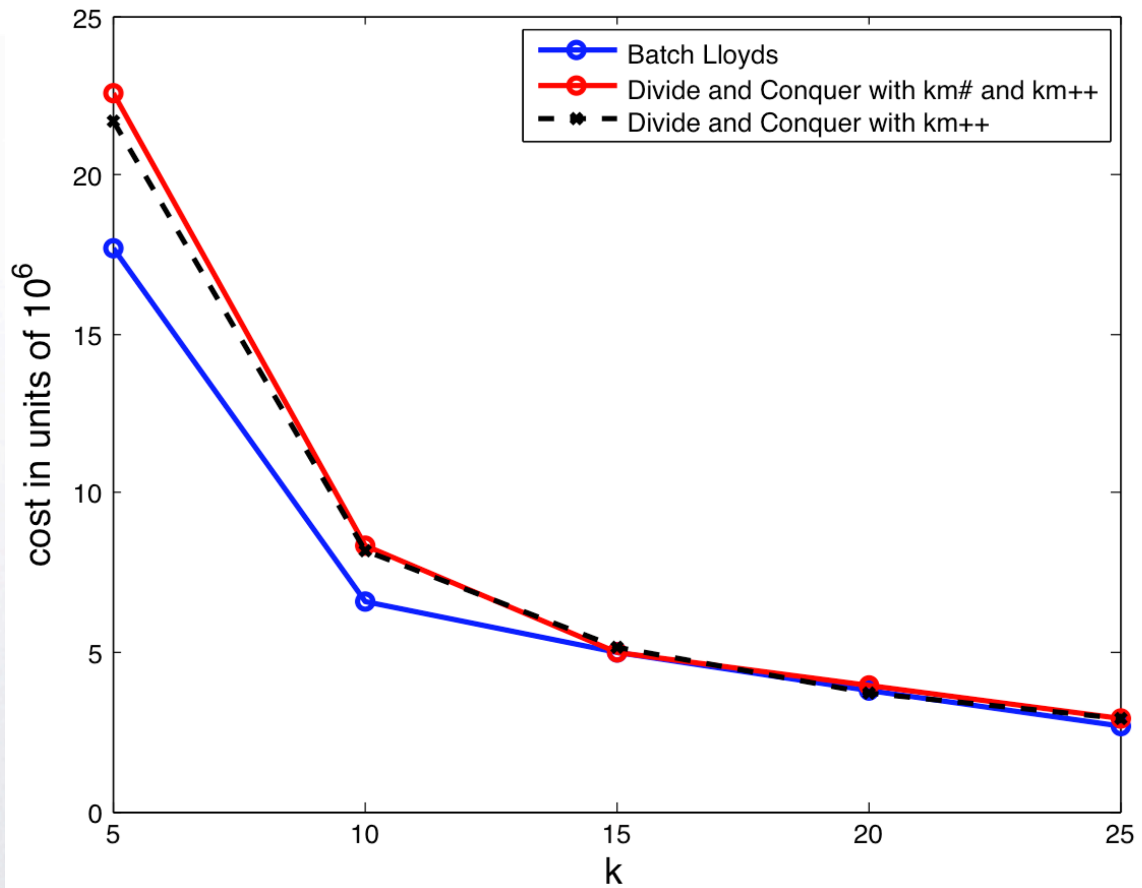
10K points sampled from a mixture of 25 Gaussians chosen at random from 15 dimensional hypercube (side 500).

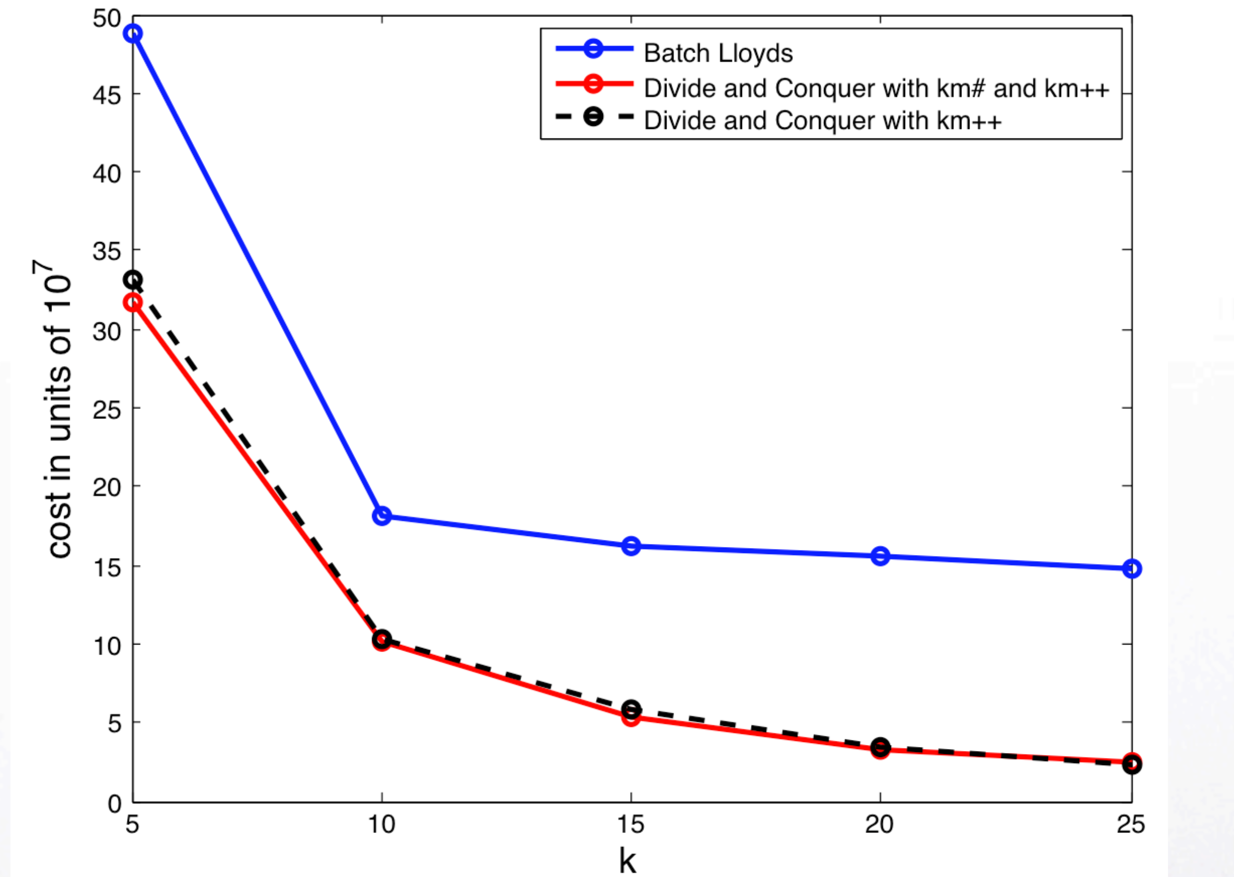


Experiments

k	BL	OL	DC-1	DC-2	BL	OL	DC-1	DC-2
5	$1.7713 \cdot 107$	$1.2401 \cdot 108$	$2.2582 \cdot 107$	$2.1683 \cdot 107$	1.78	0.15	2.30	1.10
10	$6.5871 \cdot 10^6$	$8.5684 \cdot 10^7$	$8.3452 \cdot 10^6$	$8.2037 \cdot 10^6$	2.27	0.31	7.45	2.40
15	$4.9851 \cdot 10^6$	$8.4633 \cdot 10^7$	$4.9935 \cdot 10^6$	$5.1391 \cdot 10^6$	3.42	0.45	13.34	3.32
20	$3.7836 \cdot 10^6$	$6.5110 \cdot 10^7$	$3.9289 \cdot 10^6$	$3.7279 \cdot 10^6$	3.38	0.59	32.42	5.00
25	$2.6363 \cdot 10^6$	$6.3758 \cdot 10^7$	$2.8899 \cdot 10^6$	$2.9470 \cdot 10^6$	4.54	0.62	46.45	5.89

Table 2: Cloud dataset. (columns 2-5 has the clustering cost and columns 6-9 has time in sec.)





k	BL	OL	DC-1	DC-2	BL	OL	DC-1	DC-2
5	$4.8769 \cdot 10^8$	$1.7001 \cdot 10^9$	$3.1770 \cdot 10^8$	$3.3191 \cdot 10^8$	3.74	0.87	14.60	6.53
10	$1.8169 \cdot 10^8$	$1.6930 \cdot 10^9$	$1.0104 \cdot 10^8$	$1.0271 \cdot 10^8$	5.59	1.66	47.92	12.17
15	$1.6227 \cdot 10^8$	$1.4762 \cdot 10^9$	$5.3517 \cdot 10^7$	$5.7865 \cdot 10^7$	7.04	2.19	86.54	17.53
20	$1.5580 \cdot 10^8$	$1.4766 \cdot 10^9$	$3.2577 \cdot 10^7$	$3.4155 \cdot 10^7$	9.87	2.83	218.95	25.70
25	$1.4704 \cdot 10^8$	$1.4754 \cdot 10^9$	$2.3981 \cdot 10^8$	$2.2735 \cdot 10^8$	13.26	4.41	331.77	40.64

Table 3: Spambase dataset. (columns 2-5 has the clustering cost and columns 6-9 has time in sec.)

UCI data: Clouds and Spambase.

Experiments

Memory/approximation tradeoff:

Memory/ #levels	Cost	Time	Memory/ #levels	Cost	Time	Memory/ #levels	Cost	Time
1024/0	$8.74 \cdot 10^6$	5.5	2048/0	$5.78 \cdot 10^4$	30	4601/0	$1.06 \cdot 10^8$	34
480/1	$8.59 \cdot 10^6$	3.6	1250/1	$5.36 \cdot 10^4$	25	880/1	$0.99 \cdot 10^8$	20
360/2	$8.61 \cdot 10^6$	3.8	1125/2	$5.15 \cdot 10^4$	26	600/2	$1.03 \cdot 10^8$	19.5

UCI Cloud, k=10; 25 Gaussians, k=25; UCI Spambase, k=10

Divide and conquer with *k*-means# at all levels except last, and then *k*-means++

These runs did not seem to reach a memory limit that would result in worse approximation.

Future work

Simple extensions: tightening analysis, further experimentation.

Use [Kanungo *et al.* '04] as sub-algorithm to attain a one-pass algorithm with *constant* approximation.

Analyze under data assumptions, e.g. i.i.d. or well-separated means.

Next step: an algorithm that approximates k-means in the online setting.

Thank you!

And many thanks to my coauthors:

Nir Ailon, Google Research NYC

Ragesh Jaiswal, Columbia University