Coresets for k-means clustering

Melanie Schmidt, TU Dortmund

Resource-aware Machine Learning - International Summer School

02.10.2014

Coresets and k-means

75 KB

75 KB

55 KB

75 KB

34 KB


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C: Data Volume
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A: Unifying Data Analysis
SFB 876

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A coreset represents input data

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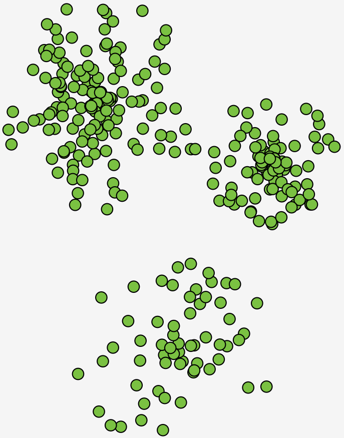
Notice that

- there is no common definition
- many approaches can be viewed as a coreset

The k-means Problem



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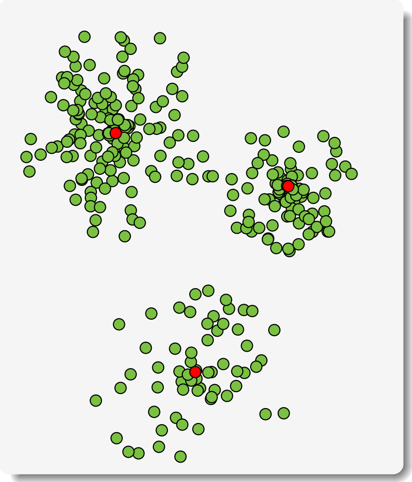

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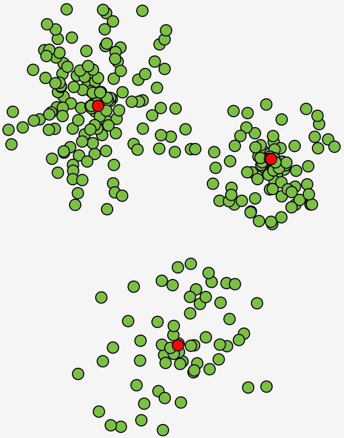

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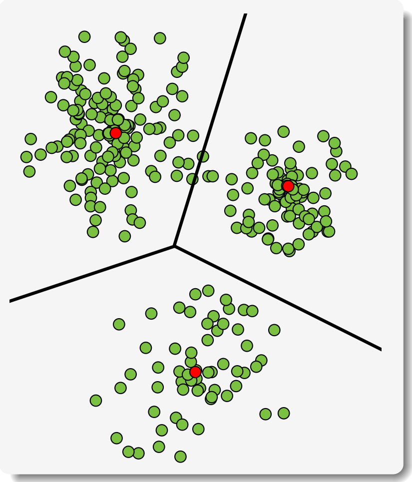
- which minimizes $\mathrm{cost}(P, C)$

$$= \sum_{p \in P} \min_{c \in C} ||c - p||^2,$$

the sum of the squared distances.



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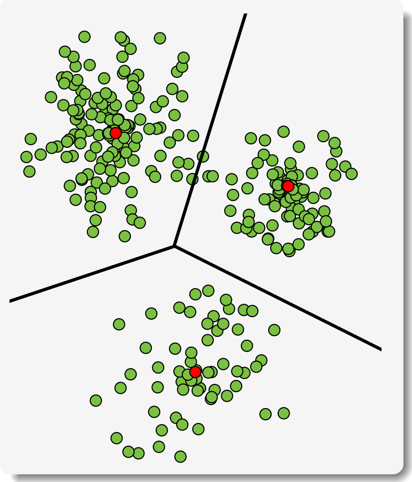

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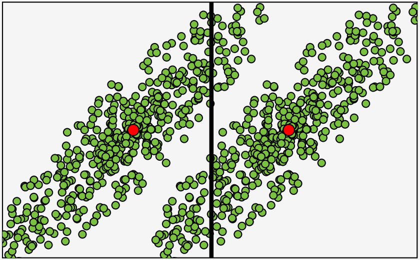
$|| \cdot ||$ is the Euclidean norm

What k-means cannot cluster



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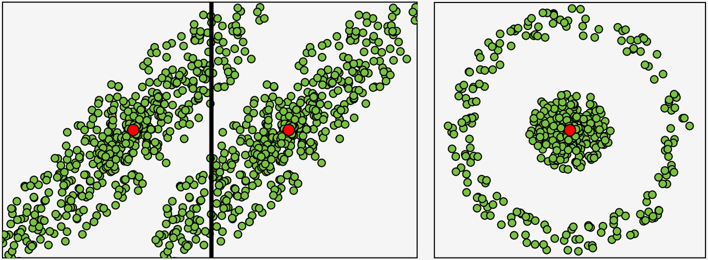

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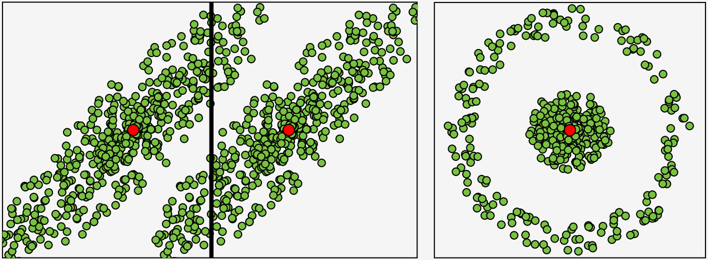

In these cases, other objective functions might be better suited

Coreset (idea)

- compute a smaller weighted point set
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- i.e., the sum of the weighted squared distances is similar
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Why for all centers?

- coreset and input should look alike for k-means

- assume optimizing over the possible centers
- if the cost is underestimated for certain center sets, then they might be mistakenly assumed to be optimal

Small summary of the data that preserves the cost function

Coresets (Har-Peled, Mazumdar)

Given a set of points $P \in \mathbb{R}^n$, a weighted set S is a (k, ϵ)-coreset if for all sets $C \subset \mathbb{R}^n$ of k centers it holds that

$$|\text{cost}_w(S, C) - \text{cost}(P, C)| \leq \epsilon \, \text{cost}(P, C)$$

where $\text{cost}_w(S, C) = \sum_{p \in S} \min_{c \in C} w(p)||p - c||^2$.

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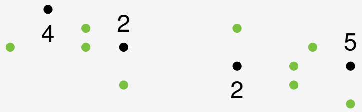

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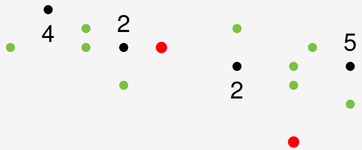

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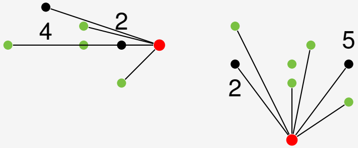

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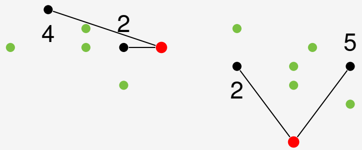


Coreset constructions

- '01: Agarwal, Har-Peled and Varadarajan: Coreset concept
- '02: Bădoiu, Har-Peled and Indyk: First coreset construction for clustering problems
- '04: Har-Peled and Mazumdar, Coreset of size $\mathcal{O}(k\epsilon^{-d} \log n)$, maintainable in data streams
- '05: Har-Peled and Kushal, Coreset of size $\mathcal{O}(k^3\varepsilon^{-(d+1)}$
- '05: Frahling and Sohler: Coreset of size $\mathcal{O}(k\epsilon^{-d} \log n)$, insertion-deletion data streams
- '06: Chen: Coresets for metric and Euclidean k-median and k-means, polynomial in d, $\log n$ and ϵ^{-1}
- '07: Feldman, Monemizadeh, Sohler: weak coreset poly(k, ϵ^{-1})
- '10: Langberg, Schulman: $\tilde{\mathcal{O}}(d^2k^3/\varepsilon^2)$
- '13: Feldman, S., Sohler: $(k/\varepsilon)^{\mathcal{O}(1)}$

Outline

- Different techniques to construct coresets
- Interlude: Dimensionality reduction
- A practically efficient coreset construction

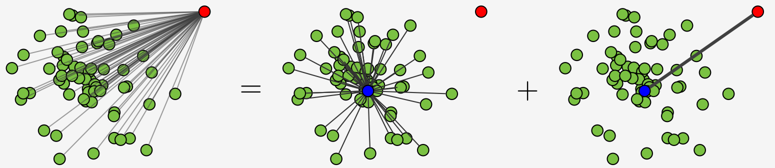
Technique 0: The magic formula for k-means

Zhang, Ramakrishnan, Livny, 1996

For every $P \subset \mathbb{R}^d$ and $z \in \mathbb{R}^d$,

$$\sum_{x \in P} ||x - z||^2 = \sum_{x \in P} ||x - \mu(P)||^2 + |P| \cdot ||\mu(P) - z||^2$$

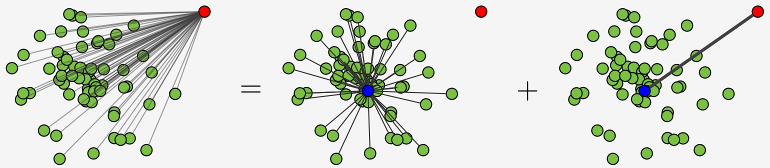
where $\mu(P) = \sum_{x \in P} x/|P|$ is the centroid of P.



Technique 0: The magic formula for k-means

Implications

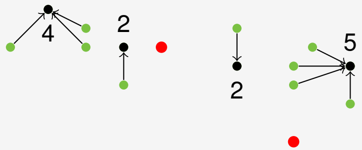
- centroid is always the optimal 1-means solution
- (much nicer situation than for 1-median!)
- centroid (plus constant) is an $(1, \varepsilon)$-coreset with no error



Technique 1: Bounded movement of points

Har-Peled, Mazumdar, 2004

- move close points to the same position
- replace coinciding points by a weighted point



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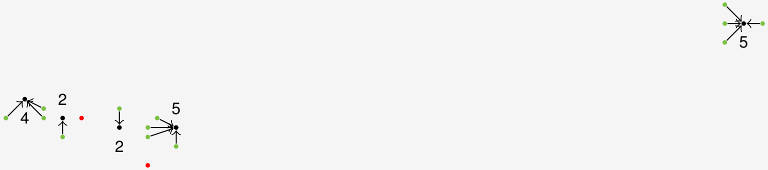

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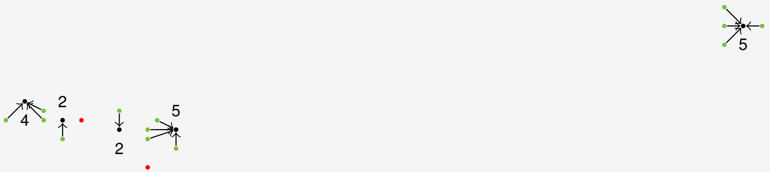

Goal

Overall squared movement small in comparison with cost

Technique 1: Bounded movement of points

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Let OPT be the cost of an optimal k-means solution.

- move each point x in P to $\pi(x)$, obtain set Q
- Ensure that

$$\sum_{x \in P} ||x - \pi(x)||^2 \leq \frac{\varepsilon^2}{16} \cdot OPT$$

- Then $|\mathrm{cost}(Q) - \mathrm{cost}(P)| \leq \varepsilon \cdot \mathrm{cost}(P)$
- $\Rightarrow \pi(P)$ is a coreset! (but a large one)

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- Move points, obtain Q, replace points by weighted points
- Notice: Sum of all movements must be small

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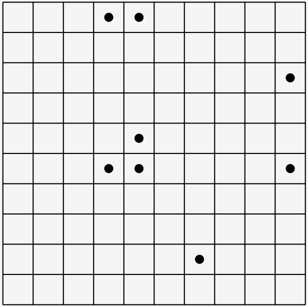

First idea:

- Place a grid
- Move all points in the same cell to one point

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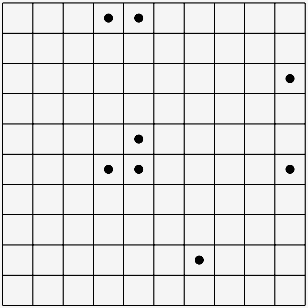

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Problem:

- Requires a cell width of $\sqrt{\varepsilon^2 OPT/(16dn)}$

$\Rightarrow$ $\Omega((nd\varepsilon^{-2})^{d/2})$ cells

- far too large ‘coreset’

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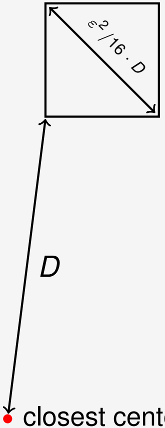

Exponential grids:

- Partition $\mathbb{R}^d$ into cells
- Goal: Small cell diameter compared to optimal clustering cost of points in the cell

$\Rightarrow$ Moving point within a cell is cheap enough

distance to center $\geq D$

$+$ cell diameter $\leq \varepsilon^2/16D$

$\Rightarrow$ movement $\leq \varepsilon^2/16\,\mathrm{cost}$

closest center in optimal solution

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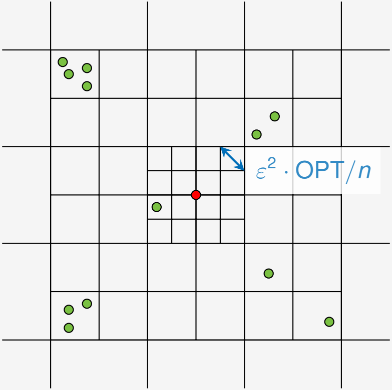

Idea

- Exponentially growing cells
- Diameter grows with distance

Construction

- An exponential grid per center
- $\mathcal{O}(\log n)$ rings in each grid
- $\mathcal{O}(\varepsilon^{-d})$ cells in each ring

$=$ $\mathcal{O}(k \log n \varepsilon^{-d})$ cells

Finally: Bicriteria approximation

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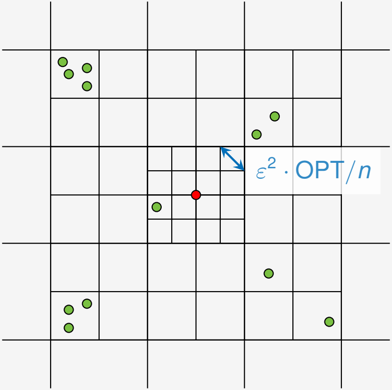

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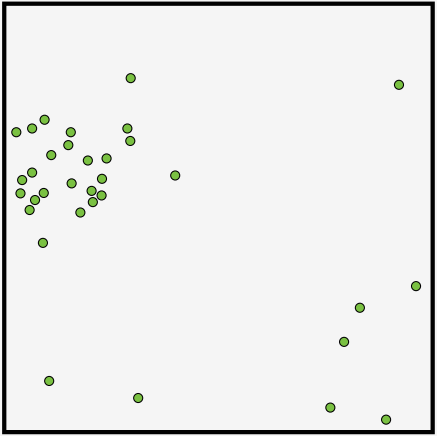
Finally: Bicriteria approximation

There exists a (k, ε)-coreset of size $\mathcal{O}(k \log^4 n/\varepsilon^d)$.

Frahling, Sohler, 2005



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- Distribute error more evenly among cells
- A cell is δ-heavy if its diameter times its number of points is $> \delta OPT$

$\Rightarrow$ smaller heavy cells contain more points

- place a coreset point in every heavy cell that has no heavy child cells

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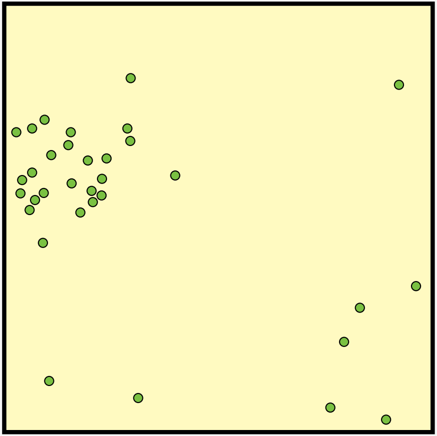

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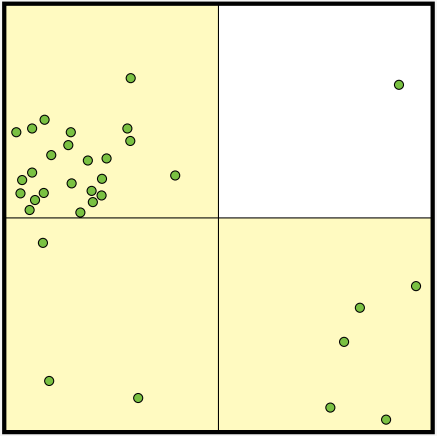

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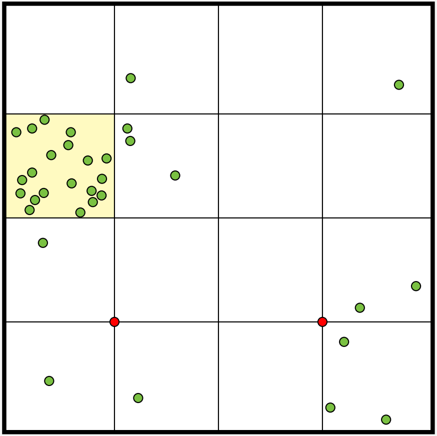

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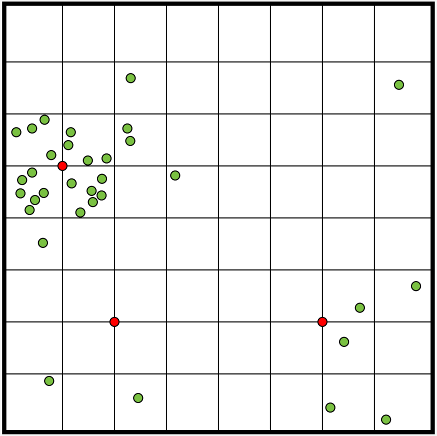

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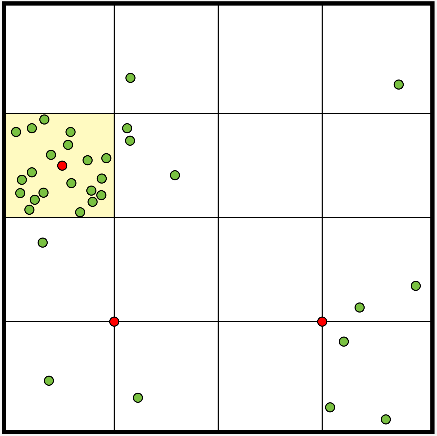

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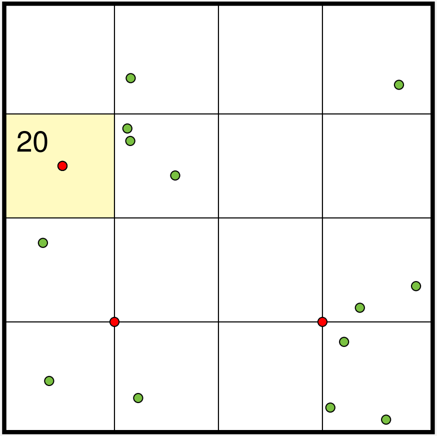

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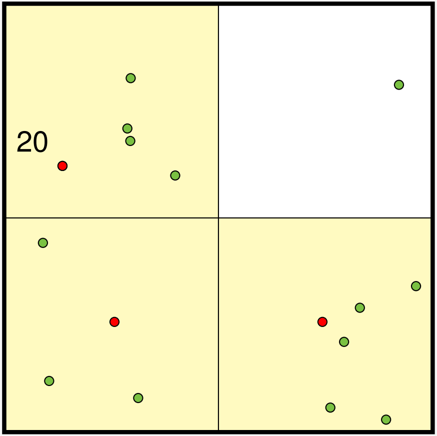

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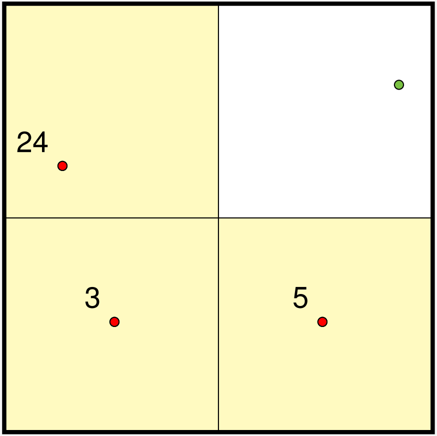

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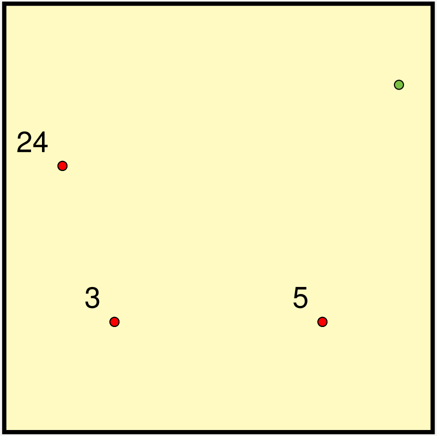

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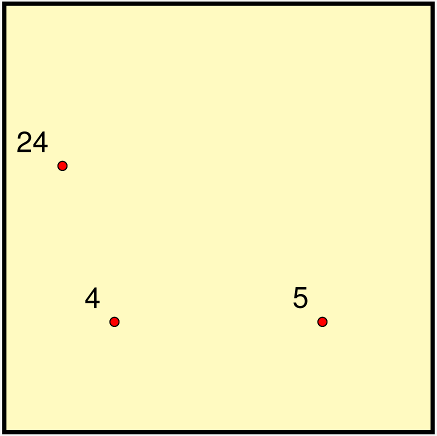

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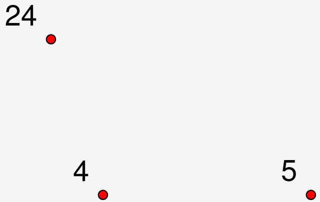

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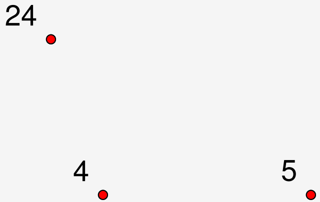

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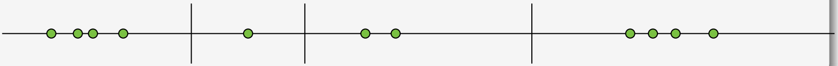
There exists a coreset of size $\mathcal{O}(k \log n \varepsilon^{-d})$.

Har-Peled, Kushal, 2005

Coreset for one-dimensional input

- Subdivide into $\mathcal{O}(k^2/\varepsilon^2)$ intervals with $\mathcal{O}((\varepsilon/k)^2 OPT)$ cost
- Place two coreset points in each interval with correct mean
- Most of the intervals are clustered with one center
- These induce no error!
- Error for remaining $k-1$ intervals can be bounded



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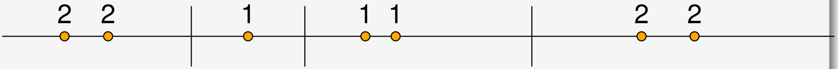

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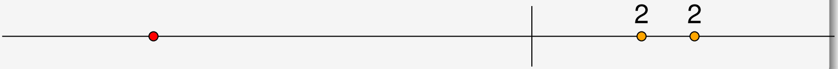

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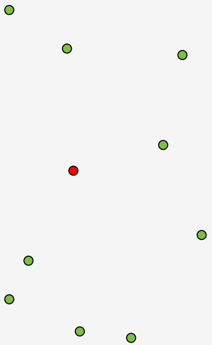

Multidimensional coreset

- Again, centers of a bicriteria approximation
- Shoot $\mathcal{O}(\varepsilon^{-(d-1)})$ rays from each center
- Project points to the rays
- Compute $\mathcal{O}(k \cdot \varepsilon^{-(d-1)})$ one-dimensional coresets

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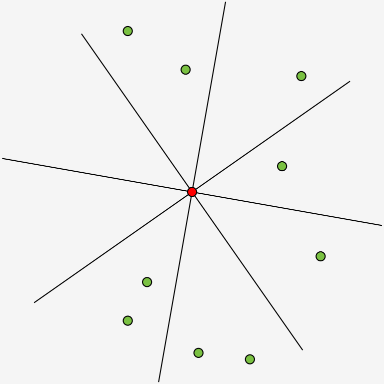

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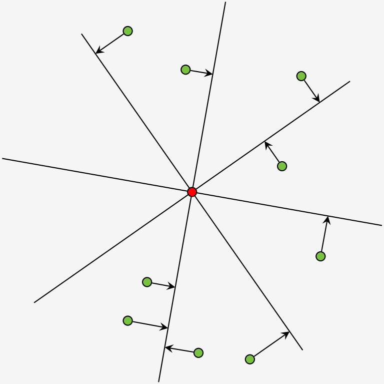

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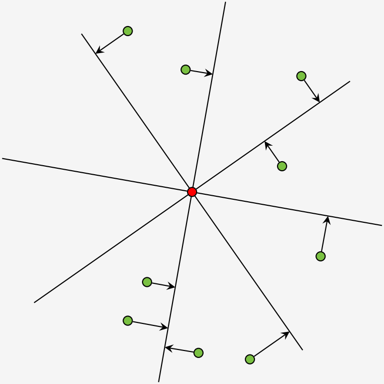

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There exists a (k, ε)-coreset of size $\mathcal{O}(k^3/\varepsilon^{d+1})$.

Technique 2: Sampling

Sampling Algorithm

- Sample points from P uniformly at random
- The sampled points form the coreset

Around $\mathcal{O}(k \cdot \log n \cdot n \cdot diam(P)/(\varepsilon^2 \cdot OPT))$ samples needed

Precise statements due to Haussler (1990),
can be proven by Hoeffding's inequality

Technique 2: Sampling

Chen, 2006

- compute bicriteria approximation
- partition input points into subsets with $\mathit{diam}(P') \approx \mathrm{cost}(P')/|P'|$
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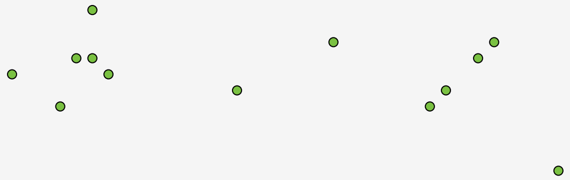

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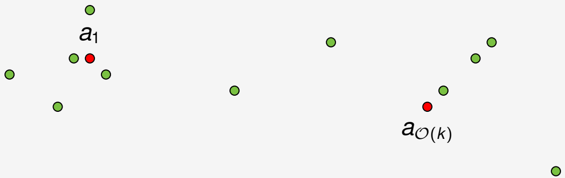

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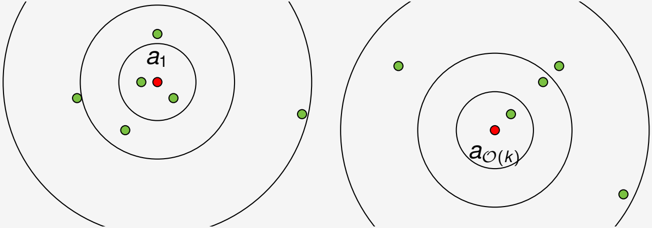

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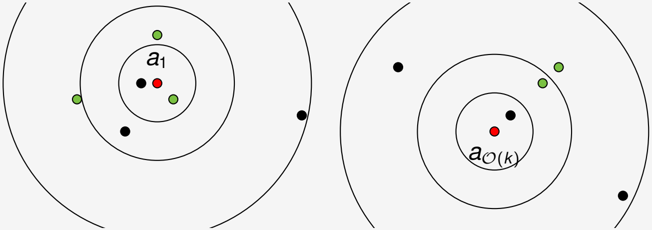

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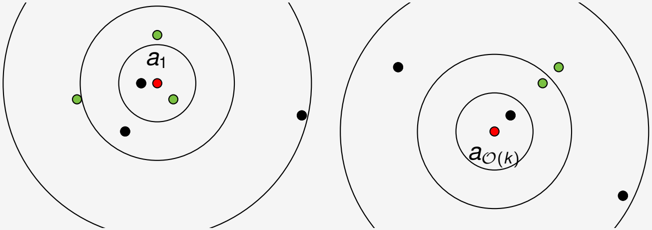

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There exists a (k, ε)-coreset of size $\widetilde{\mathcal{O}}(dk^2 \log n/\varepsilon^2)$.

Technique 2: Refined sampling strategies

Feldman, Monemizadeh, Sohler, 2007

Importance sampling

- Sample points with a probability proportional to their optimum cost
- Weight points accordingly
- For points with low optimum cost, sample uniformly

Improvement due to Langberg, Schulman, 2010.

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Technique 2: Refined sampling strategies

Feldman, Langberg, 2011

Sensitivity based sampling

- The sensitivity of a point $x \in P$ is

$$\sup_{C \subset \mathbb{R}^d, |C|=k} \frac{\min_{c \in C} ||x - c||^2}{\sum_{y \in P} \min_{c \in C} ||y - c||^2}$$

- Maximum share of a point in the cost function

$\Rightarrow$ Sampling probabilities proportional to sensitivity

Technique 3: Pseudorandomness

Idea

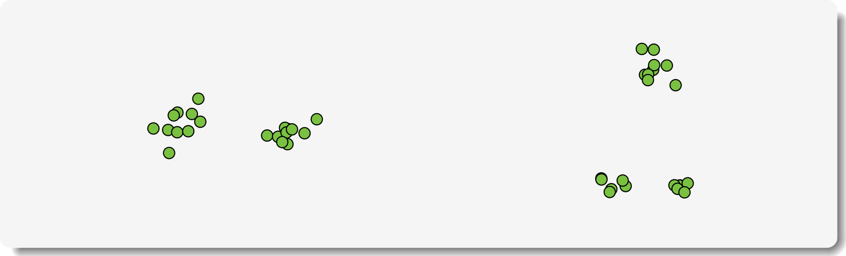
- If a point set has little structure (it is pseudorandom), clustering it is similar for all centers

$\Rightarrow$ Clustering it with one center does not induce much error

$\Rightarrow$ Simulate clustering with one center by using the centroid

Partition the input into pseudorandom subsets

Technique 3: Pseudorandomness



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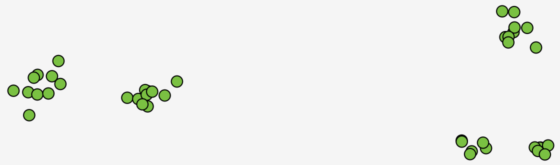

- Start with partitioning according to an optimal center set
- Continiously subdivide sets until every set S satisfies:
- Clustering S with k centers is at most a factor $(1 + \epsilon)$ cheaper than clustering S with one center

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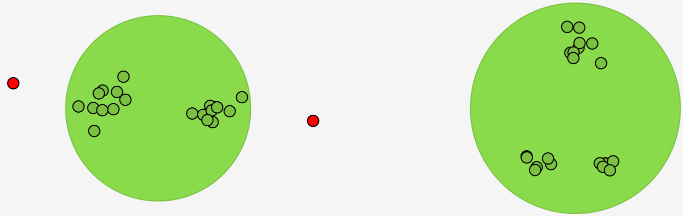

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- . . . or cost for 1-clustering is negligible $(\varepsilon^2 OPT)$

Technique 3: Pseudorandomness

- sets on level 1 together cost OPT
- sets on level i cost $\frac{OPT}{(1+\epsilon)^i}$
- sets on level $\log_{1+\epsilon} \epsilon^{-2}$ have negligible cost ($\epsilon^2 OPT$)
- $\mathcal{O}\left(k^{\log_{1+\epsilon} \epsilon^{-2}}\right)$ coreset points $\rightarrow$ independent of n and d

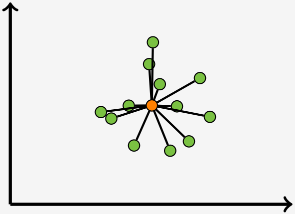
Technique 4: Dimensionality reduction

Drineas, Frieze, Kannan, Vempala, Vinay, 1999

Let P be a set of n points in $\mathbb{R}^n$. Consider the best fit subspace

$$V_k := \arg \min_{\dim(V)=k} \sum_{p \in P} d(p, V)^2 \subset \mathbb{R}^n.$$

Solving the projected instance in V_k yields a 2-approximation.



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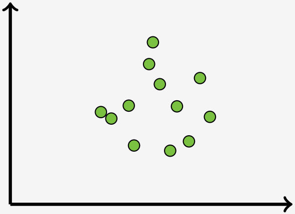

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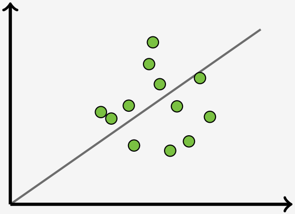

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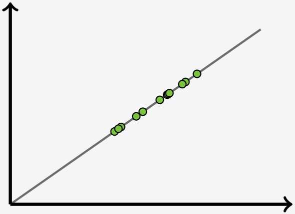

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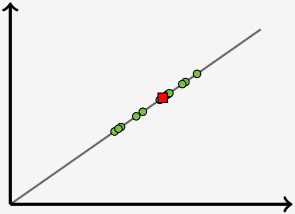

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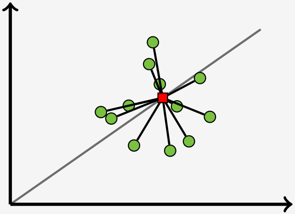

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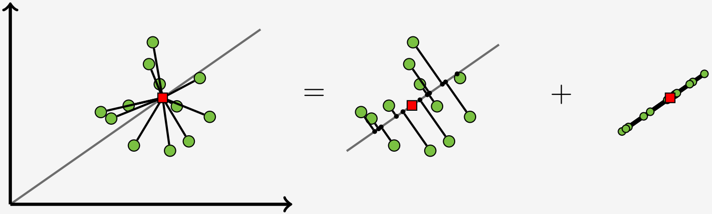

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Feldman, S., Sohler, 2013

Projecting to $V_{\mathcal{O}(k/\epsilon^2)}$ instead yields a $(1+\epsilon)$-approximation.

There exists a coreset of size $\tilde{\mathcal{O}}(k^4\varepsilon^{-4})$.

Processing Big Data

- Most coreset constructions need random access
- Undesirable / not possible for Big Data or streaming settings

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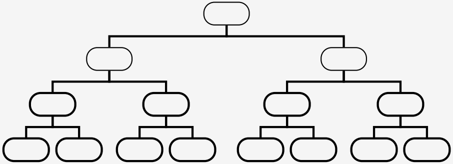
Conversion to a Streaming Algorithm: Merge & Reduce



- read data in blocks
- compute a coreset for each block $\rightarrow s$
- merge coresets in a tree fashion
- $\rightsquigarrow$ space $s \cdot \log n$

Coreset sizes increase, algorithm has additional overhead

Streaming coreset algorithms (no Merge & Reduce)

- Coreset construction due to Frahling and Sohler
- BICO (Fichtenberger, Gillé, S., Schwiegelshohn, Sohler)

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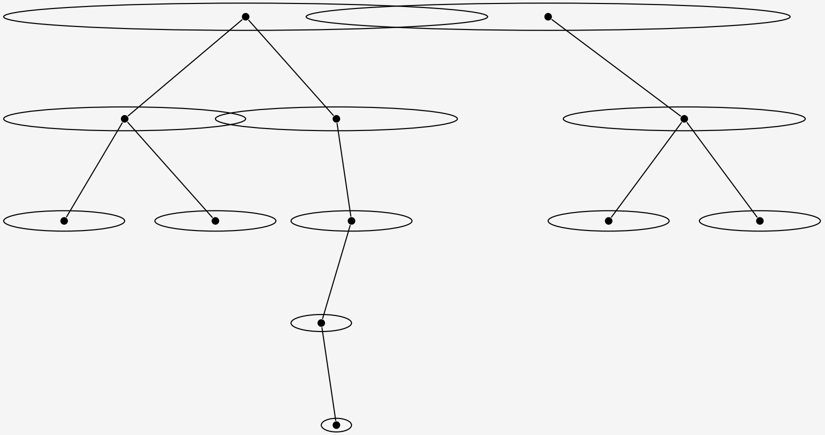
BICO

- based on the datastructure of BIRCH
- works with Technique 1 (bounded movement of points)
- computes a coreset
- `http://ls2-www.cs.tu-dortmund.de/bico`

BIRCH

- Zhang, Ramakrishnan, Livny, 1997
- SIGMOD Test of Time Award 2006

A practically efficient coreset algorithm



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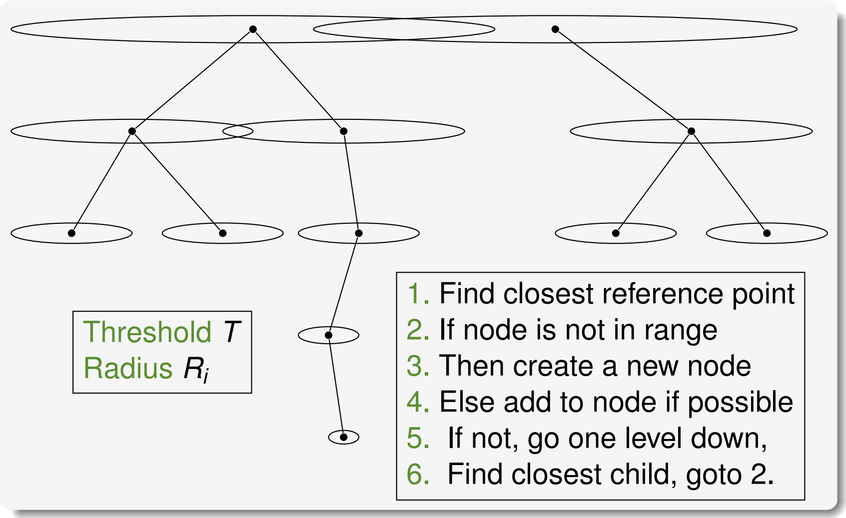

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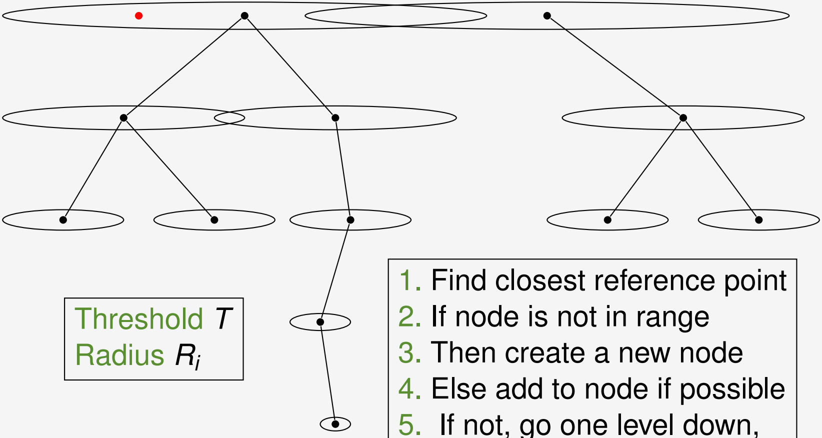

1. Find closest reference point
2. If node is not in range
3. Then create a new node
4. Else add to node if possible
5. If not, go one level down,
6. Find closest child, goto 2.

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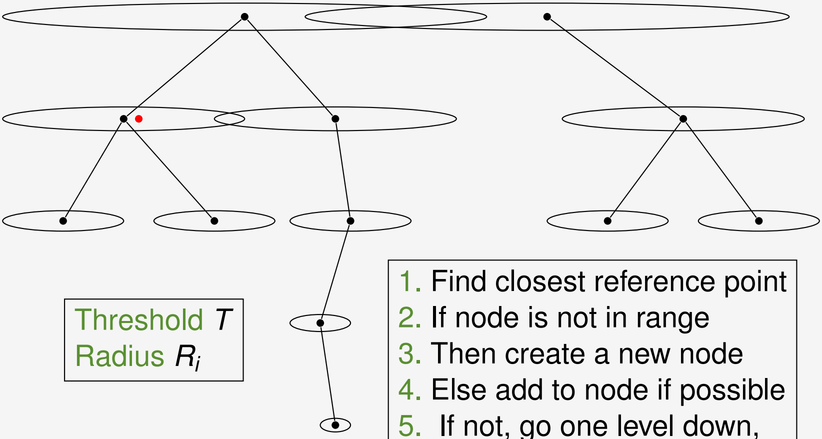

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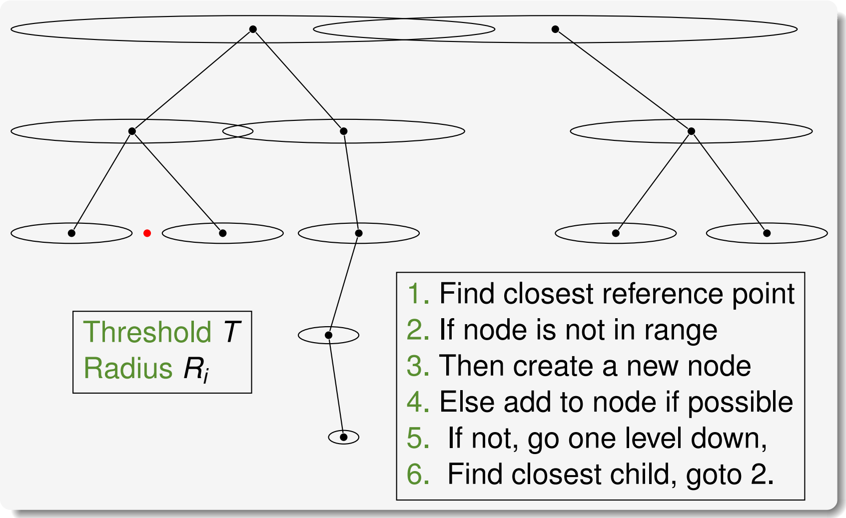

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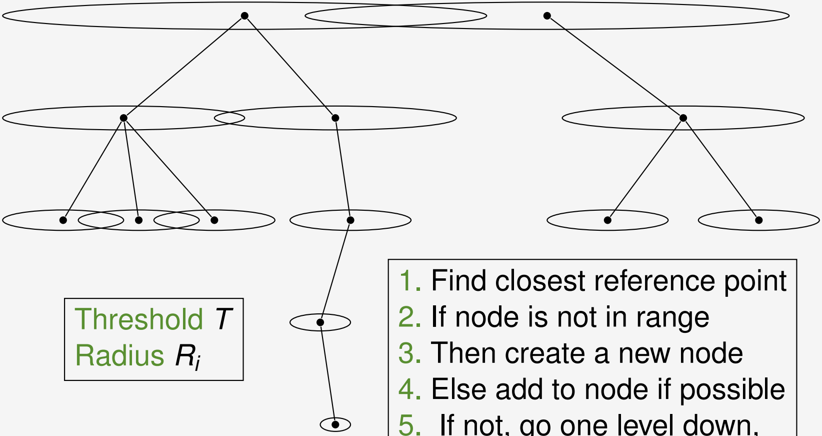

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Algorithms for comparison

- StreamKM++ and BIRCH (author's implementations)
- MacQueen's k–means algorithm (ESMERALDA)

Data sets

	BigCross	CalTech128	Census	CoverType	Tower
n	$1 \cdot 10^7$	$3 \cdot 10^6$	$2 \cdot 10^6$	$6 \cdot 10^5$	$5 \cdot 10^6$
d	57	128	68	55	3
nd	$7 \cdot 10^8$	$4 \cdot 10^8$	$2 \cdot 10^8$	$3 \cdot 10^7$	$1 \cdot 10^7$

Diagrams

- 100 runs for every test instance
- Values shown in the diagrams are mean values

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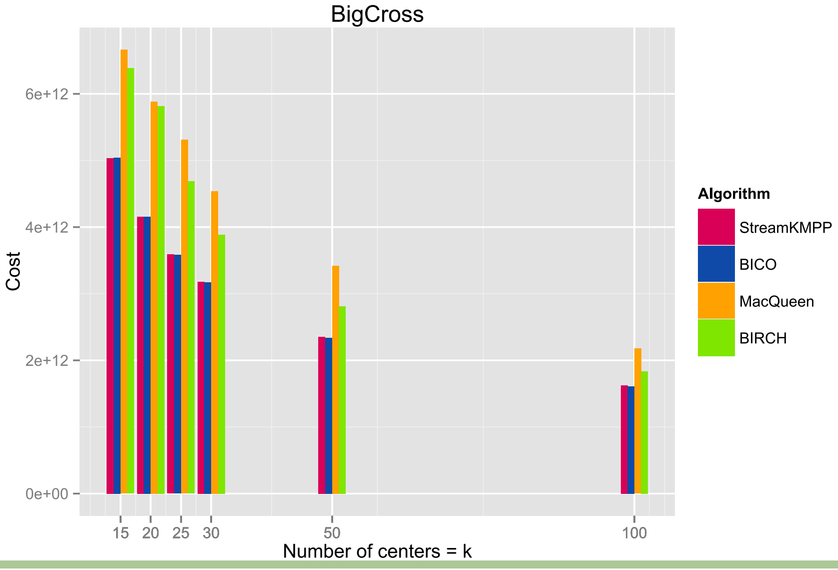

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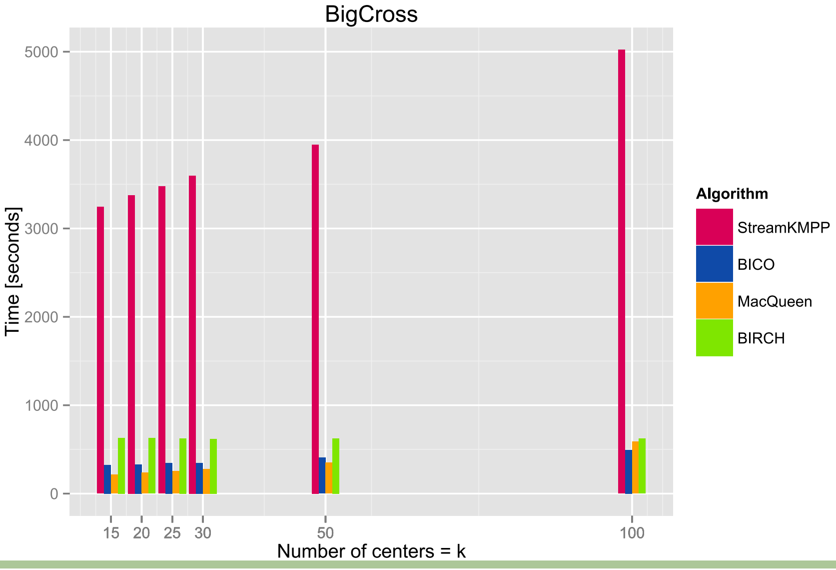

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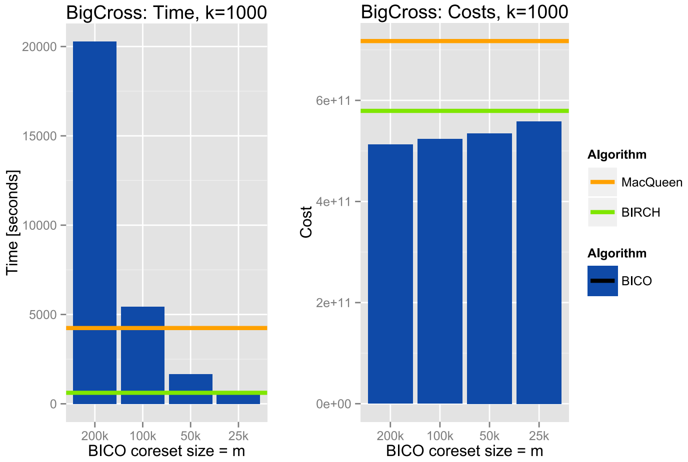

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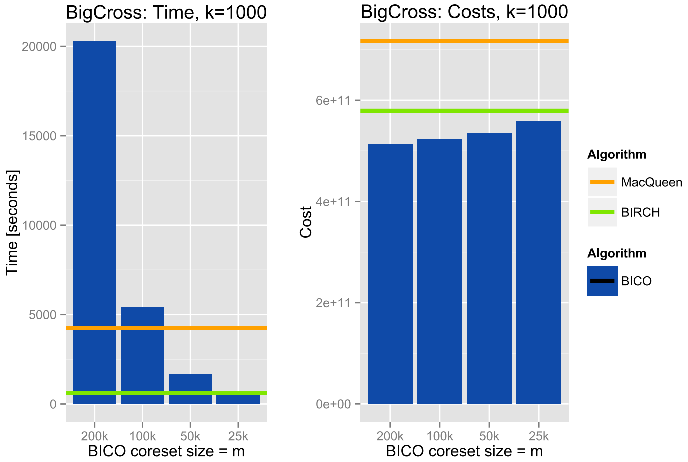

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