Clustering Methods: Part 2b

Cut-based & divisive clustering

Pasi Fränti

17.3.2014

Speech & Image Processing Unit
School of Computing
University of Eastern Finland
Joensuu, FINLAND

UNIVERSITY OF
EASTERN FINLAND

Part I:
Cut-based clustering

Cut-based clustering

- What is cut?
- Can we used graph theory in clustering?
- Is normalized-cut useful?
- Are cut-based algorithms efficient?

Clustering method

- Clustering method = defines the problem
- Clustering algorithm = solves the problem
- Problem defined as cost function
  - Goodness of one cluster
  - Similarity vs. distance
  - Global vs. local cost function (what is “cut”)
- Solution: algorithm to solve the problem

Cut-based clustering

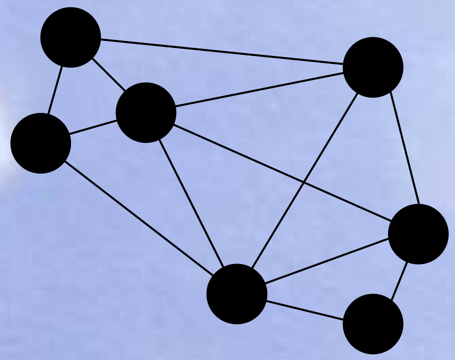
- Usually assumes graph
- Based on concept of cut
- Includes implicit assumptions which are often:
  - No difference than clustering in vector space
  - Implies sub-optimal heuristics
  - Sometimes even false assumptions!

Cut-based clustering methods

- Minimum-spanning tree based clustering (single link)
- Split-and-merge (Lin&Chen TKDE 2005): Split the data set using K-means, then merge similar clusters based on Gaussian distribution cluster similarity.
- Split-and-merge (Li, Jiu, Cot, PR 2009): Splits data into a large number of subclusters, then remove and add prototypes until no change.
- DIVFRP (Zhong et al, PRL 2008): Dividing according to furthest point heuristic.
- Normalized-cut (Shi&Malik, PAMI-2000): Cut-based, minimizing the disassociation between the groups and maximizing the association within the groups.
- Ratio-Cut (Hagen&Kahng, 1992)
- Mcut (Ding et al, ICDM 2001)
- Max k-cut (Frieze&Jerrum 1997)
- Feng et al, PRL 2010. Particle Swarm Optimization for selecting the hyperplane.

Details to be added later…

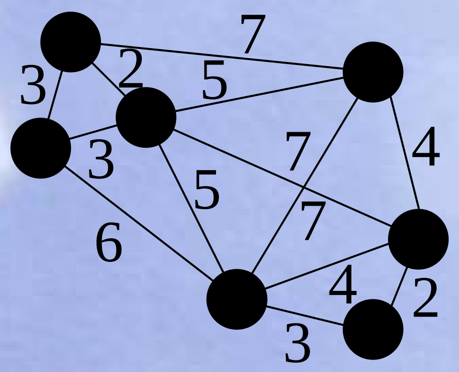
Clustering a graph



But where we
get this…?

Distance graph

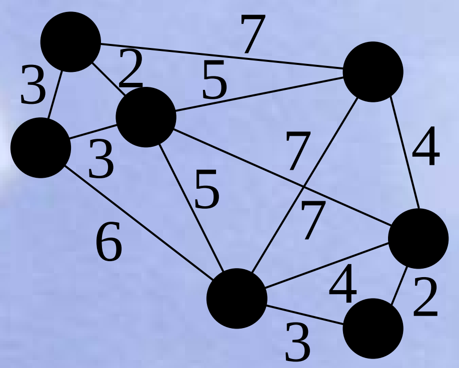
Distance graph



Calculate from vector space!

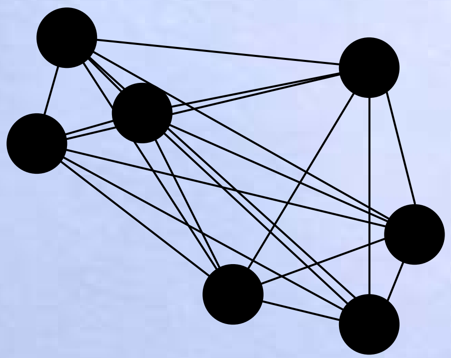
Space complexity of graph

Distance graph



But…

Complete graph

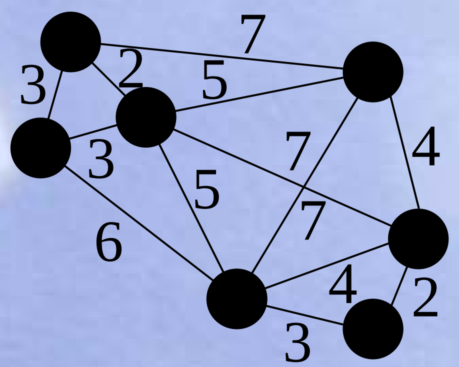


$N \cdot (N-1)/2$ edges

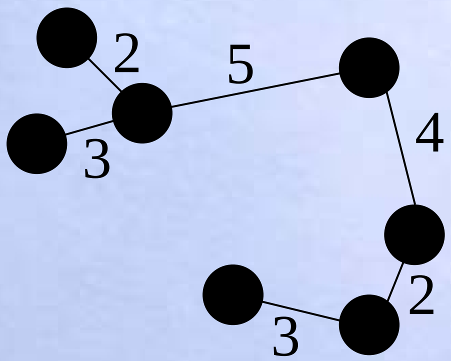
$= O(N^2)$

Minimum spanning tree (MST)

Distance graph



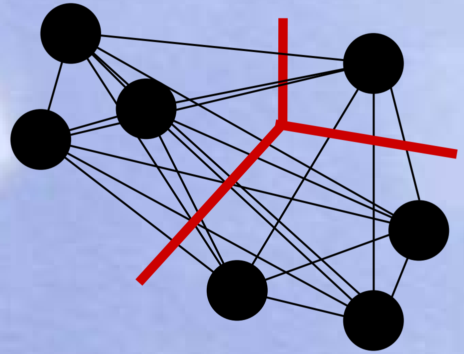
MST



Works with simple examples like this

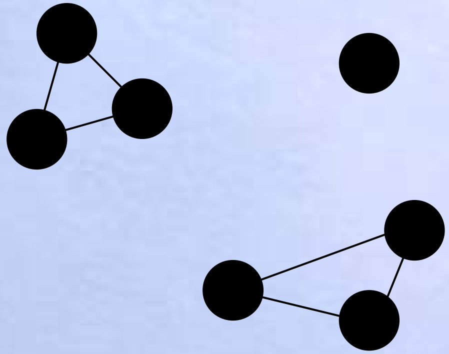
Cut

Graph cut



Cost function is to maximize the weight of edges cut

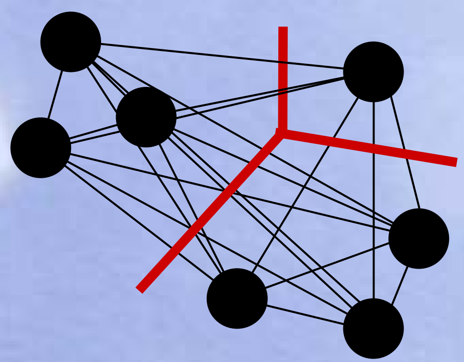
Resulted clusters



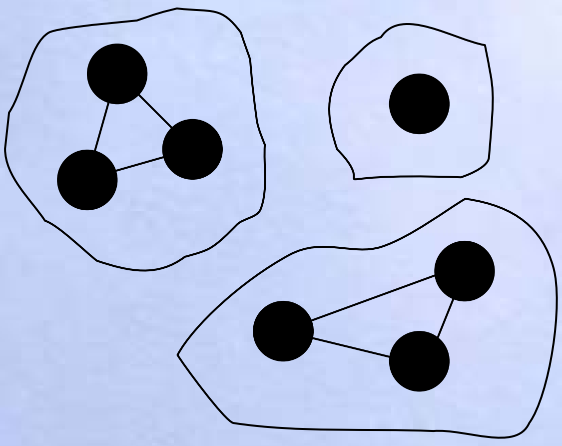
This equals to minimizing the within cluster edge weights

Cut

Graph cut



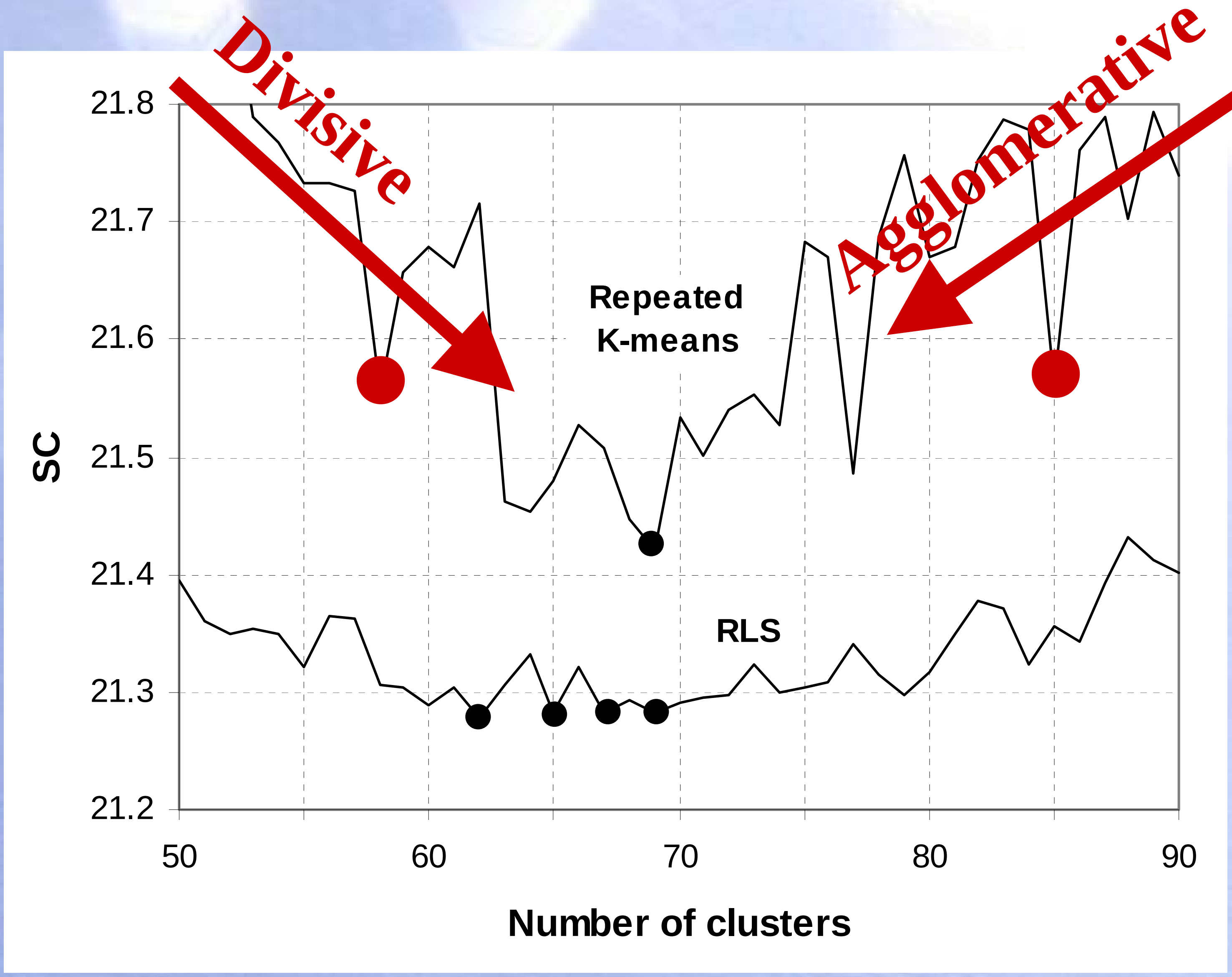
Resulted clusters



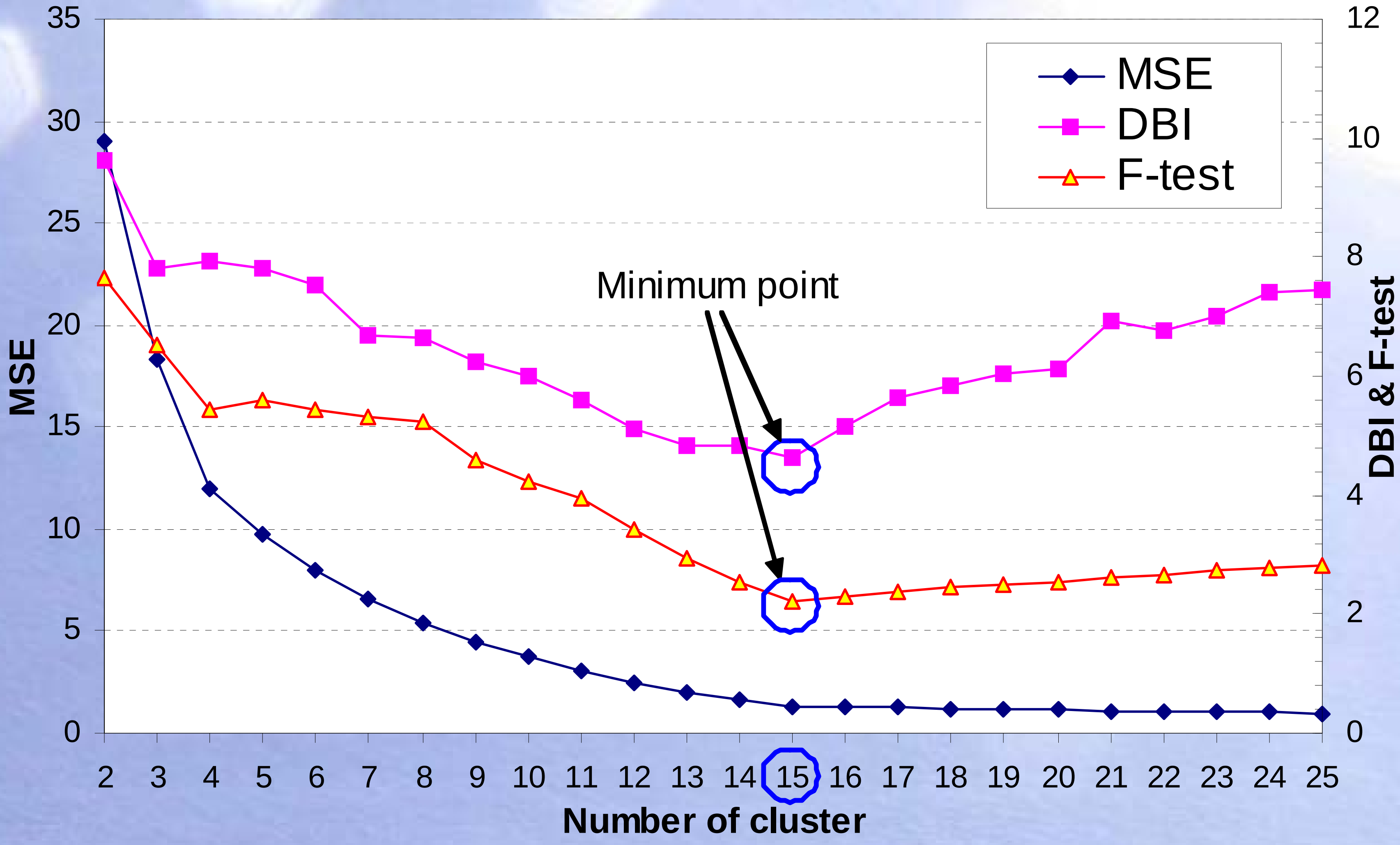
Equivalent to minimizing MSE!

Stopping criterion

Ends up to a local minimum ●

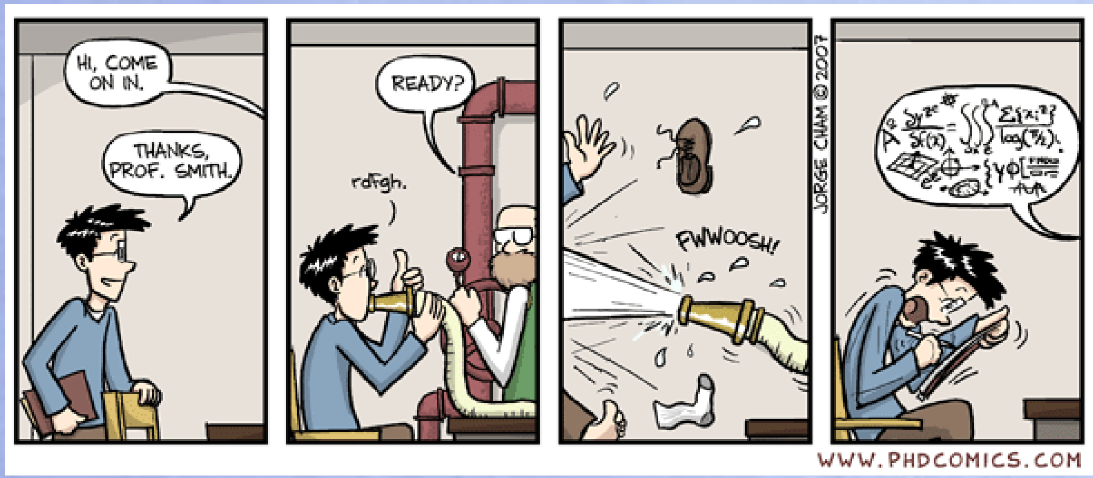


Clustering method



Conclusions of "Cut"

- Cut ⇒ Same as partition
- Cut-based method ⇒ Empty concept
- Cut-based algorithm ⇒ Same as divisive
- Graph-based clustering ⇒ Flawed concept
- Clustering of graph ⇒ more relevant topic



Part II:
Divisive algorithms

Divisive approach

Motivation

- Efficiency of divide-and-conquer approach
- Hierarchy of clusters as a result
- Useful when solving the number of clusters

Challenges

- Design problem 1: What cluster to split?
- Design problem 2: How to split?
- Sub-optimal local optimization at best

Split-based (divisive) clustering

Split(X, M) $\rightarrow$ C, P

$m \leftarrow 1$;

REPEAT

Select cluster to be split;

Split the cluster;

$m \leftarrow m+1$;

UpdateDataStructures;

UNTIL $m=M$;

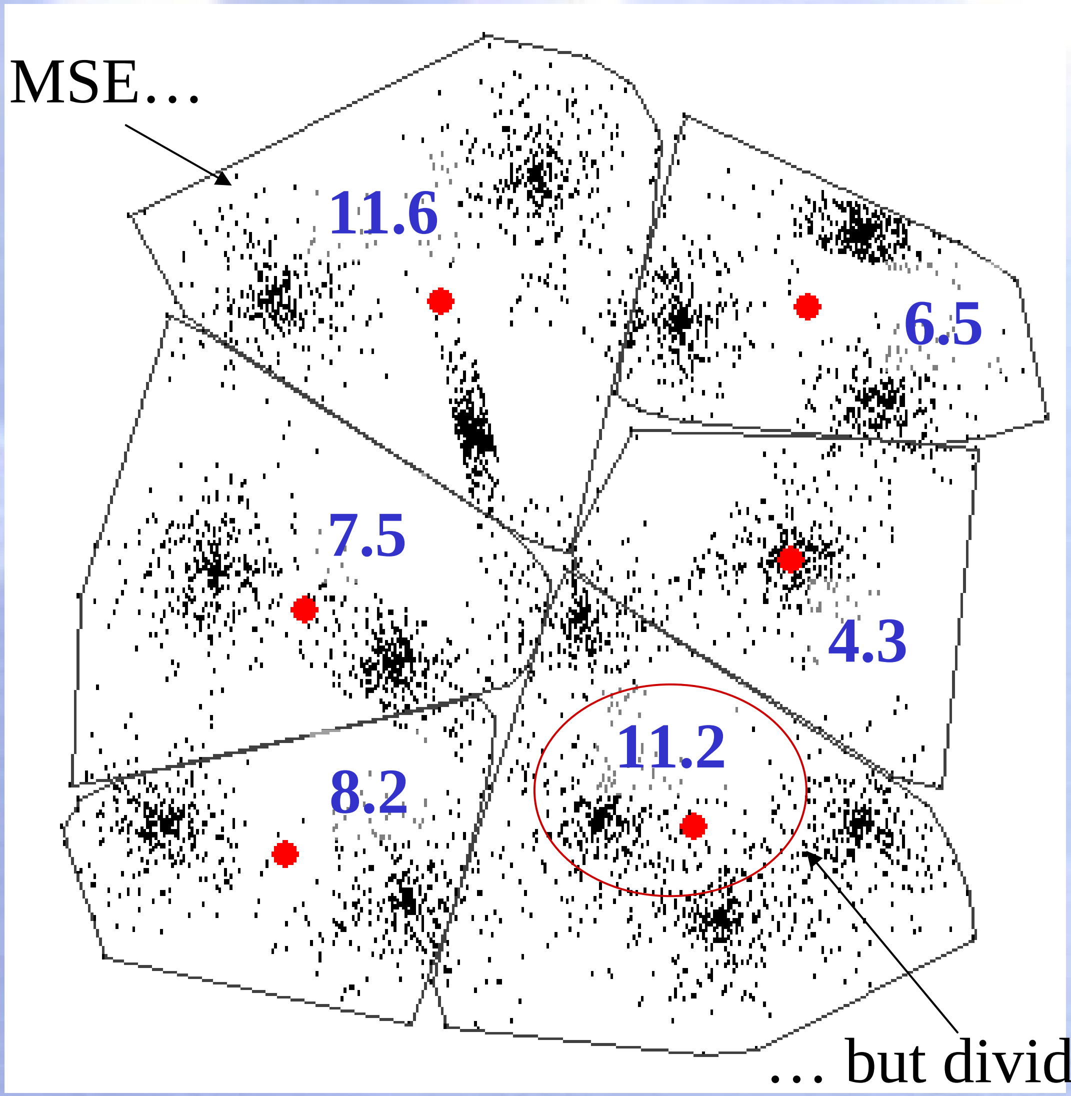
Select cluster to be split

- Heuristic choices:
  - Cluster with highest variance (MSE)
  - Cluster with most skew distribution (3rd moment)
- Optimal choice:
  - Tentatively split all clusters
  - Select the one that decreases MSE most!
- Complexity of choice:
  - Heuristics take the time to compute the measure
  - Optimal choice takes only twice (2×) more time!!!
  - The measures can be stored, and only two new clusters appear at each step to be calculated.

Use this !

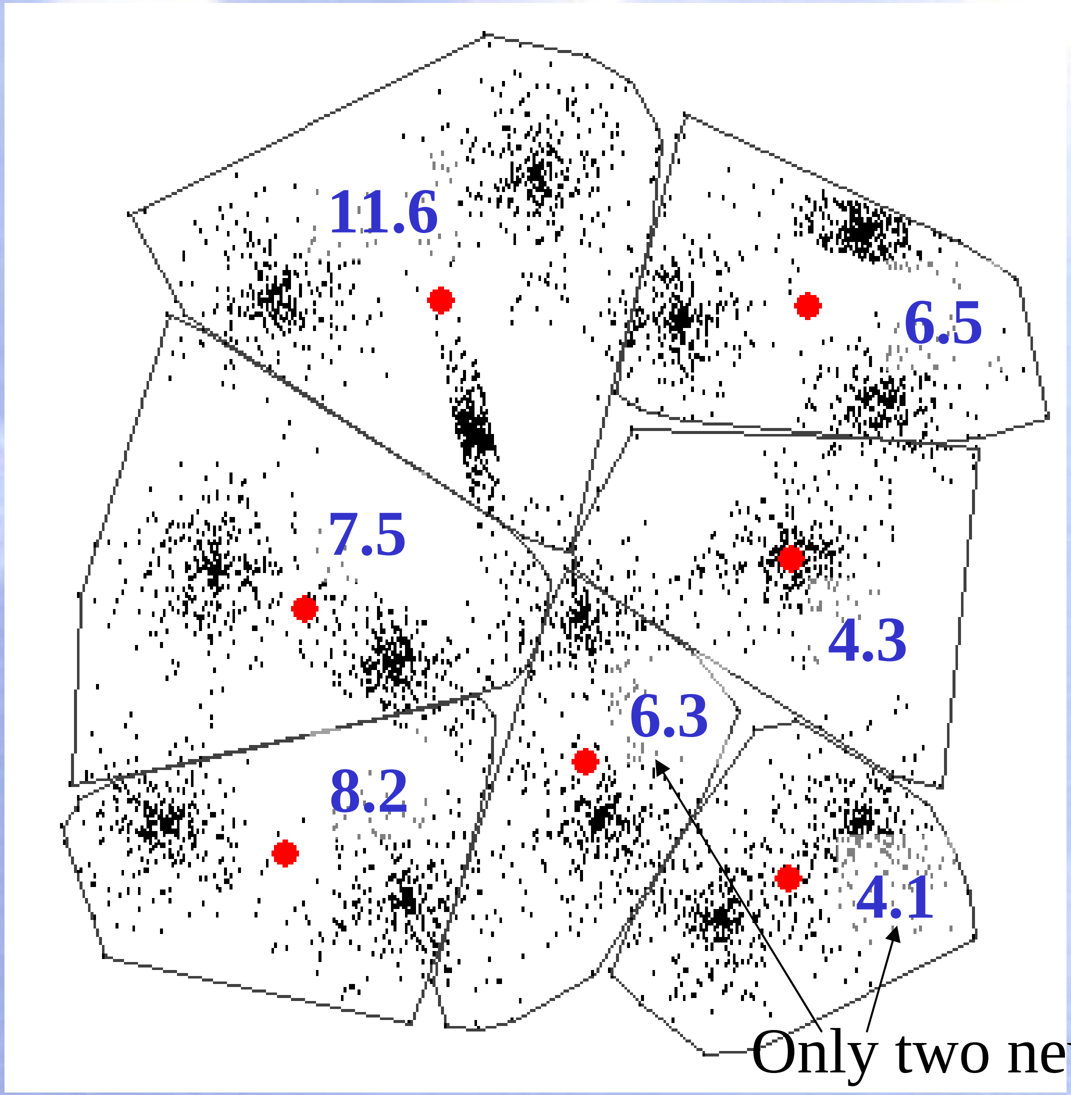
Selection example

Biggest MSE…



… but dividing this decreases MSE more

Selection example



Only two new values
need to be calculated

How to split

- Centroid methods:
  - Heuristic 1: Replace C by C-ε and C+ε
  - Heuristic 2: Two furthest vectors.
  - Heuristic 3: Two random vectors.
- Partition according to principal axis:
  - Calculate principal axis
  - Select dividing point along the axis
  - Divide by a hyperplane
  - Calculate centroids of the two sub-clusters

Splitting along principal axis

pseudo code

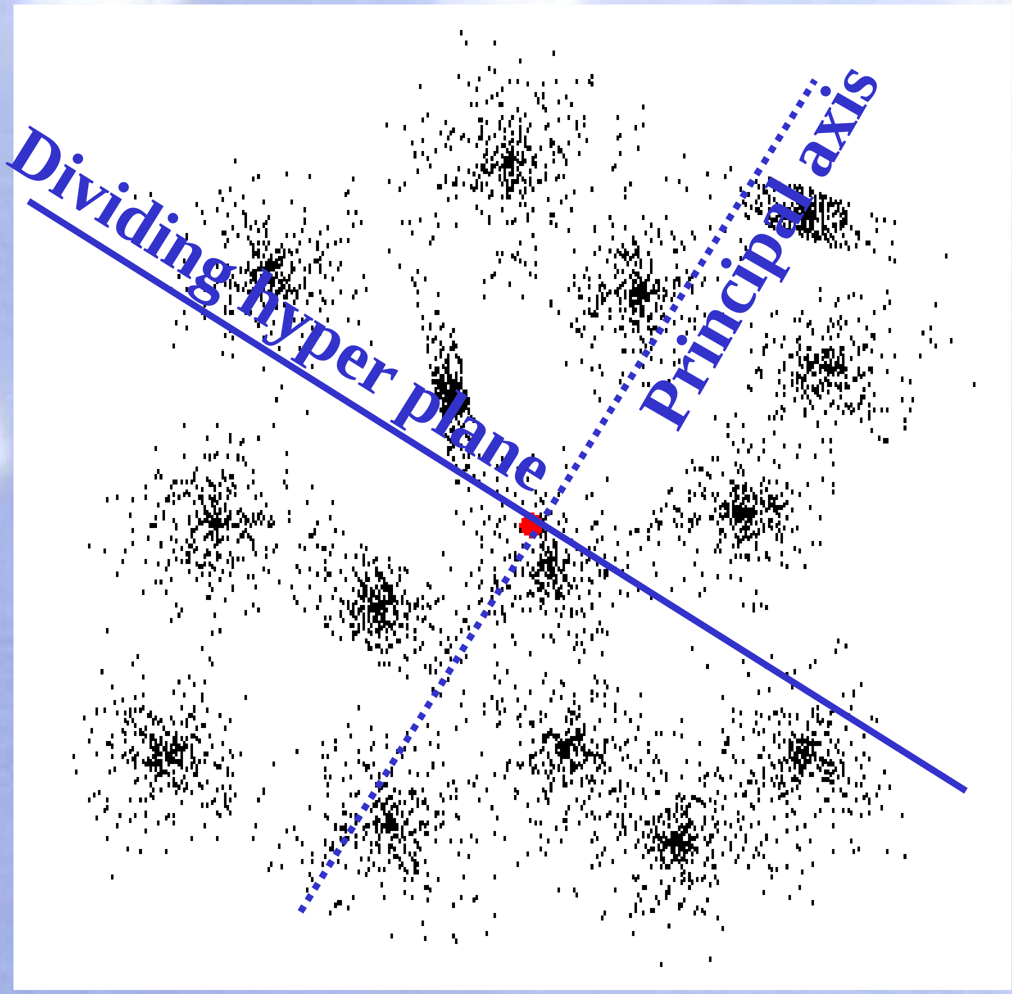
Step 1: Calculate the principal axis.

Step 2: Select a dividing point.

Step 3: Divide the points by a hyper plane.

Step 4: Calculate centroids of the new clusters.

Example of dividing



Optimal dividing point

pseudo code of Step 2

Step 2.1: Calculate projections on the principal axis.

Step 2.2: Sort vectors according to the projection.

Step 2.3: FOR each vector x_i DO:

- Divide using x_i as dividing point.
- Calculate distortion of subsets D_1 and D_2.

Step 2.4: Choose point minimizing D_1+D_2.

Finding dividing point

- Calculating error for next dividing point:

$$D' = D + \frac{n_1}{n_1 + 1} \cdot \left| c_1 - v_i \right|^2 - \frac{n_2}{n_2 - 1} \cdot \left| c_2 - v_i \right|^2$$

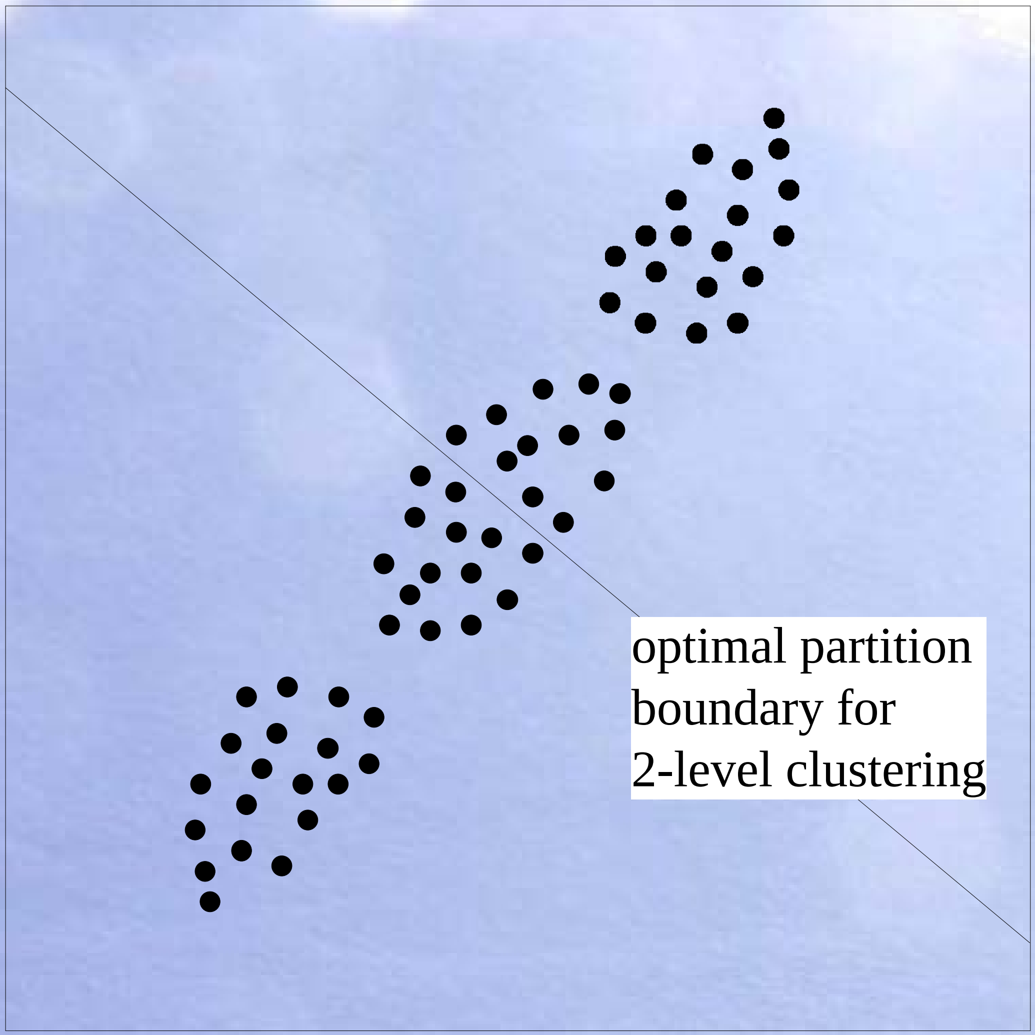
- Update centroids:

$$c_1' = \frac{n_1 c_1 + v_i}{n_1 + 1}$$

$$c_2' = \frac{n_2 c_2 - v_i}{n_2 - 1}$$

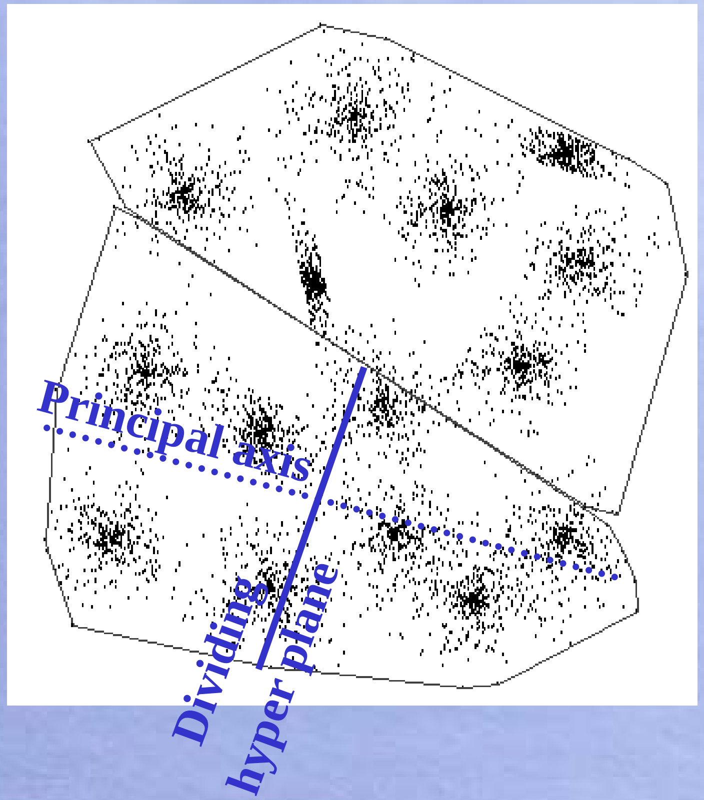
Can be done in O(1) time!!!

Sub-optimality of the split

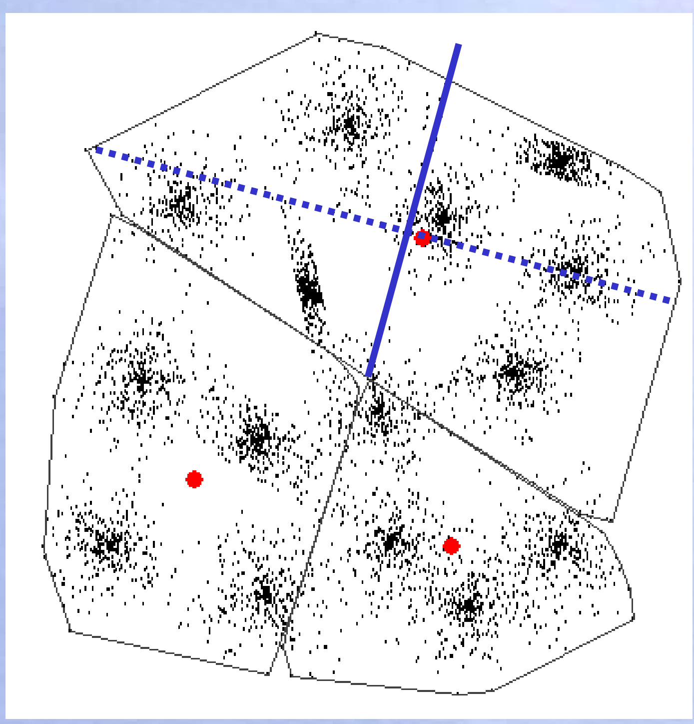


Example of splitting process

2 clusters

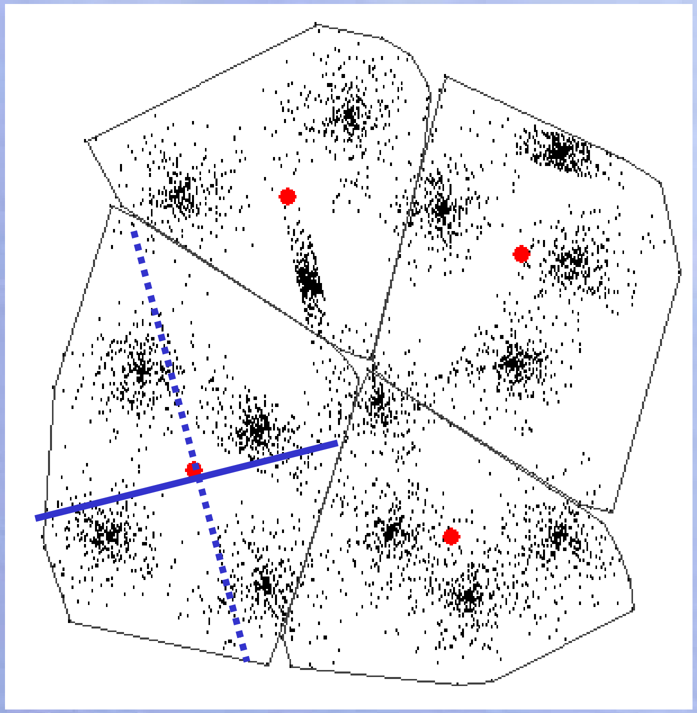


3 clusters

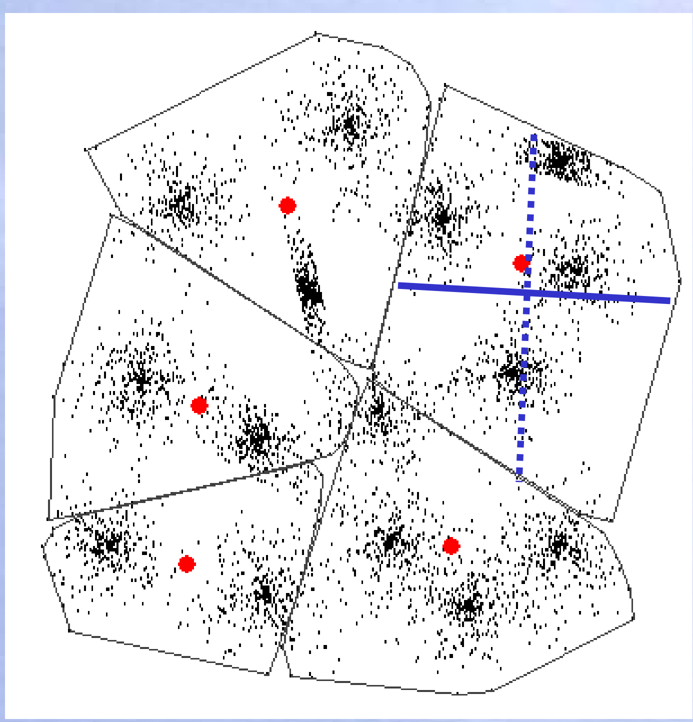


Example of splitting process

4 clusters

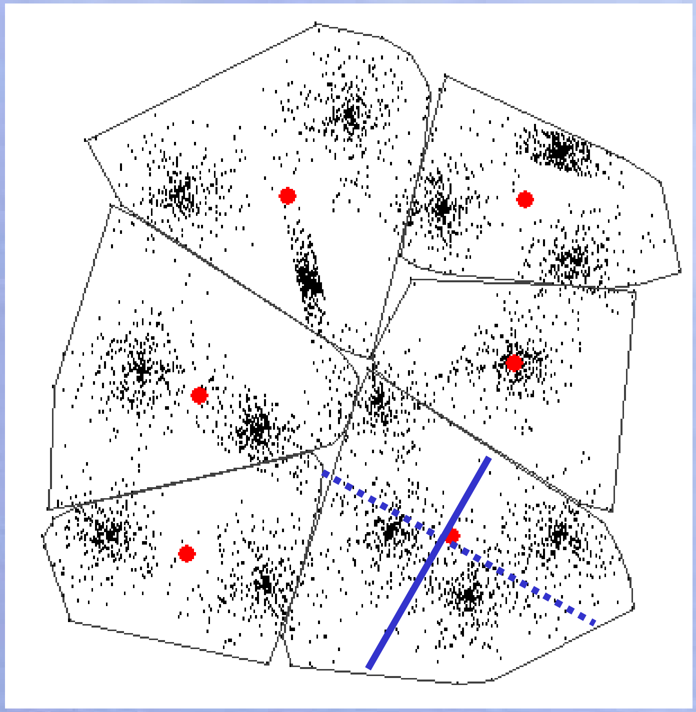


5 clusters

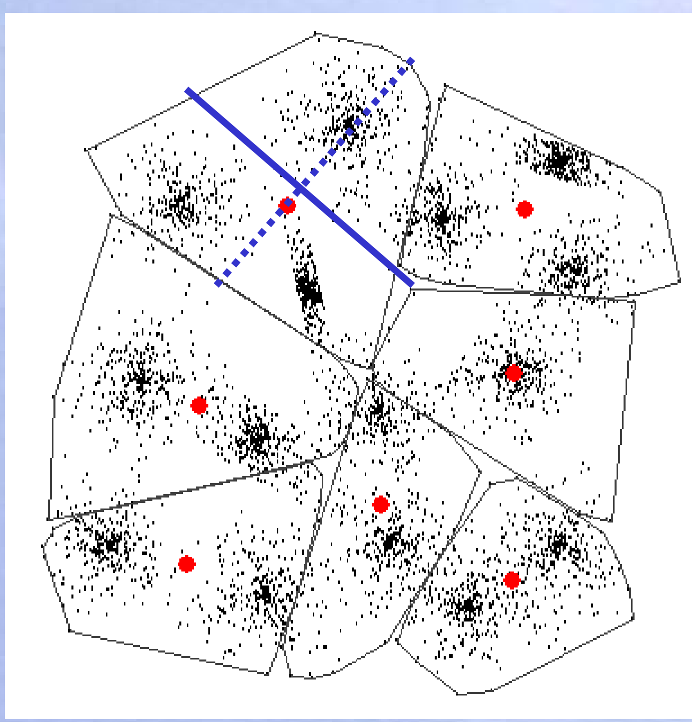


Example of splitting process

6 clusters

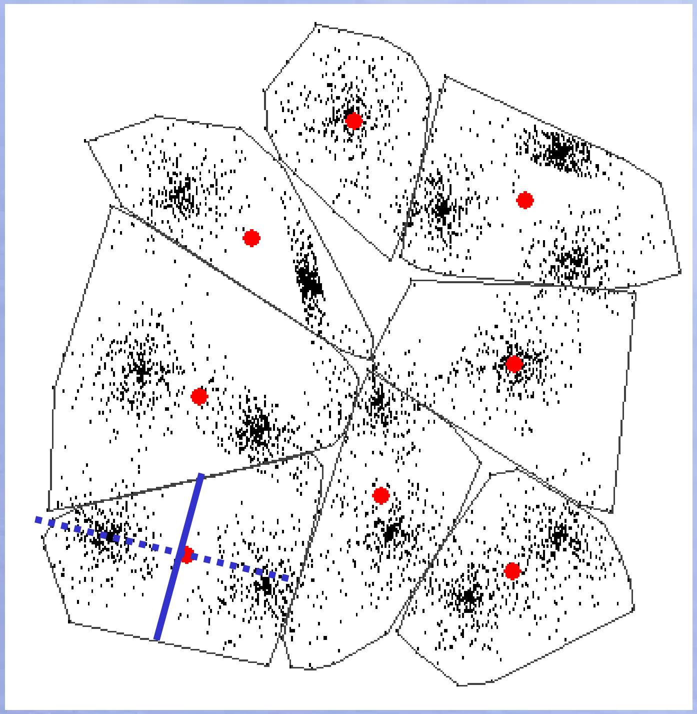


7 clusters

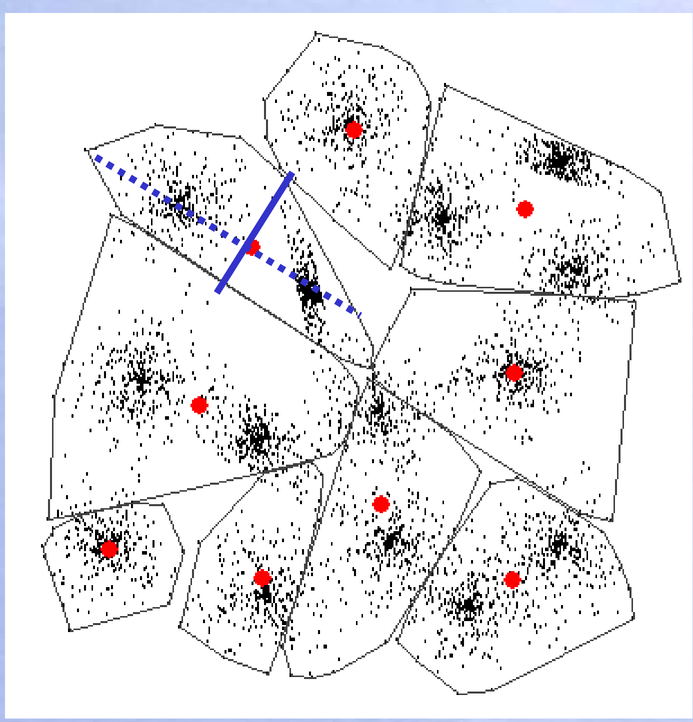


Example of splitting process

8 clusters

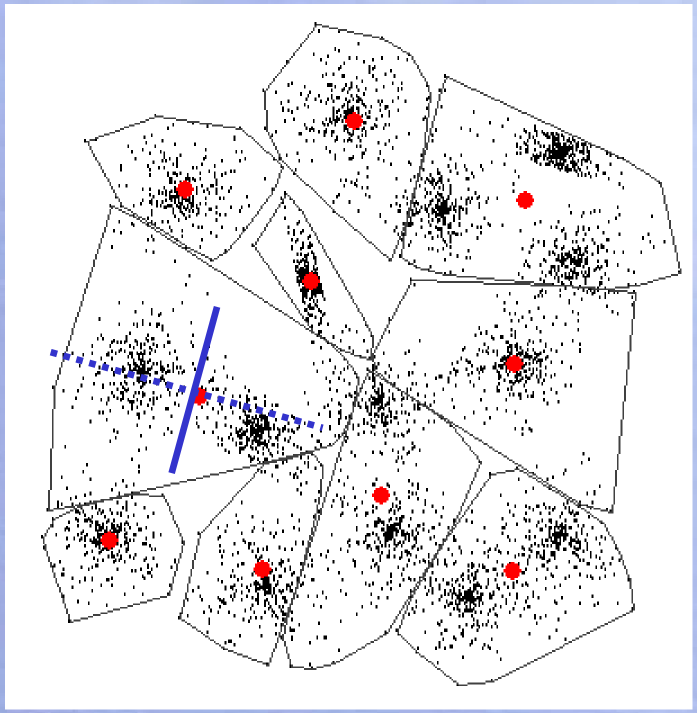


9 clusters

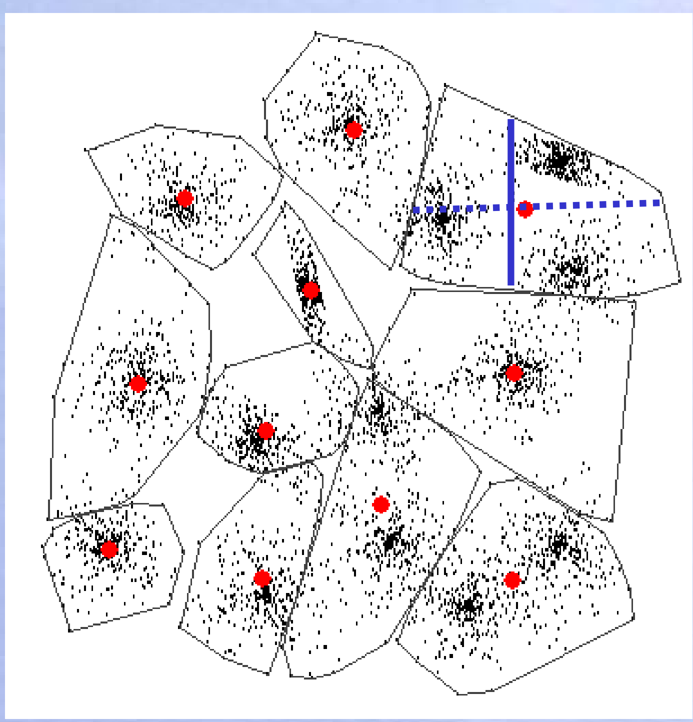


Example of splitting process

10 clusters

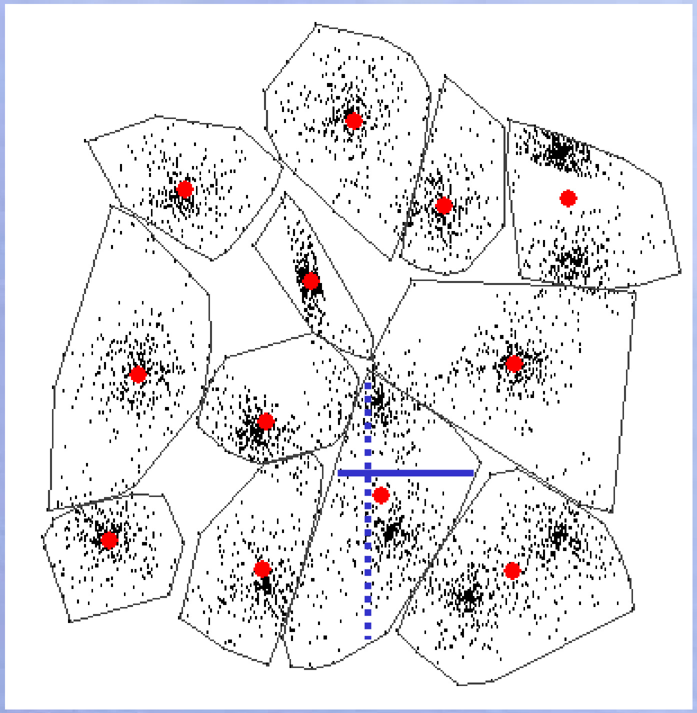


11 clusters

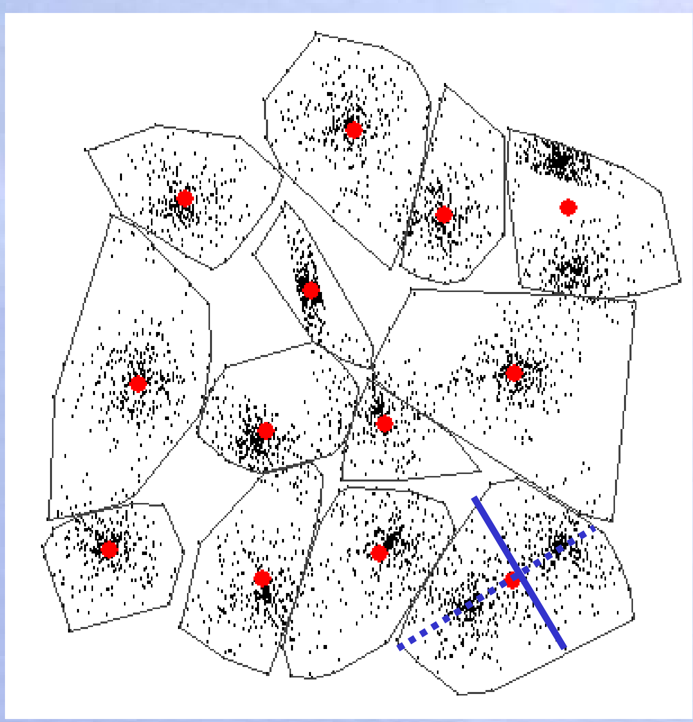


Example of splitting process

12 clusters

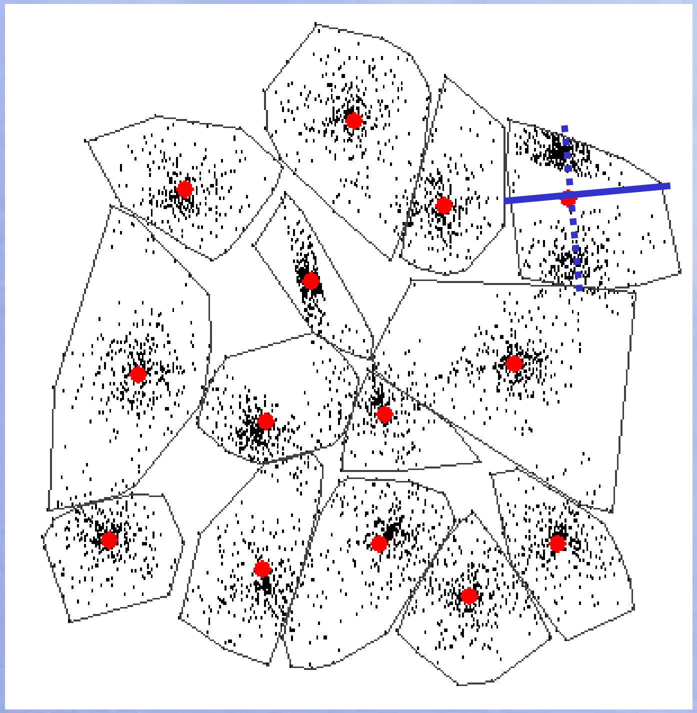


13 clusters

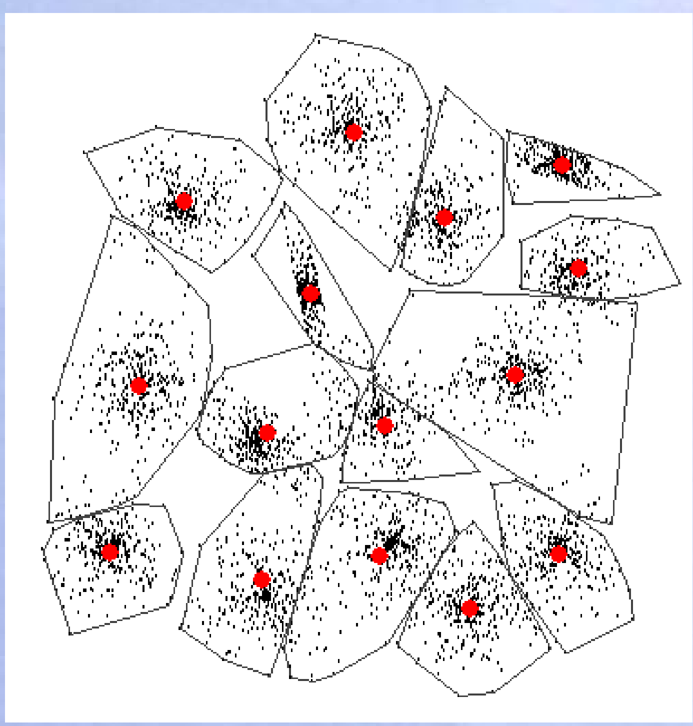


Example of splitting process

14 clusters



15 clusters



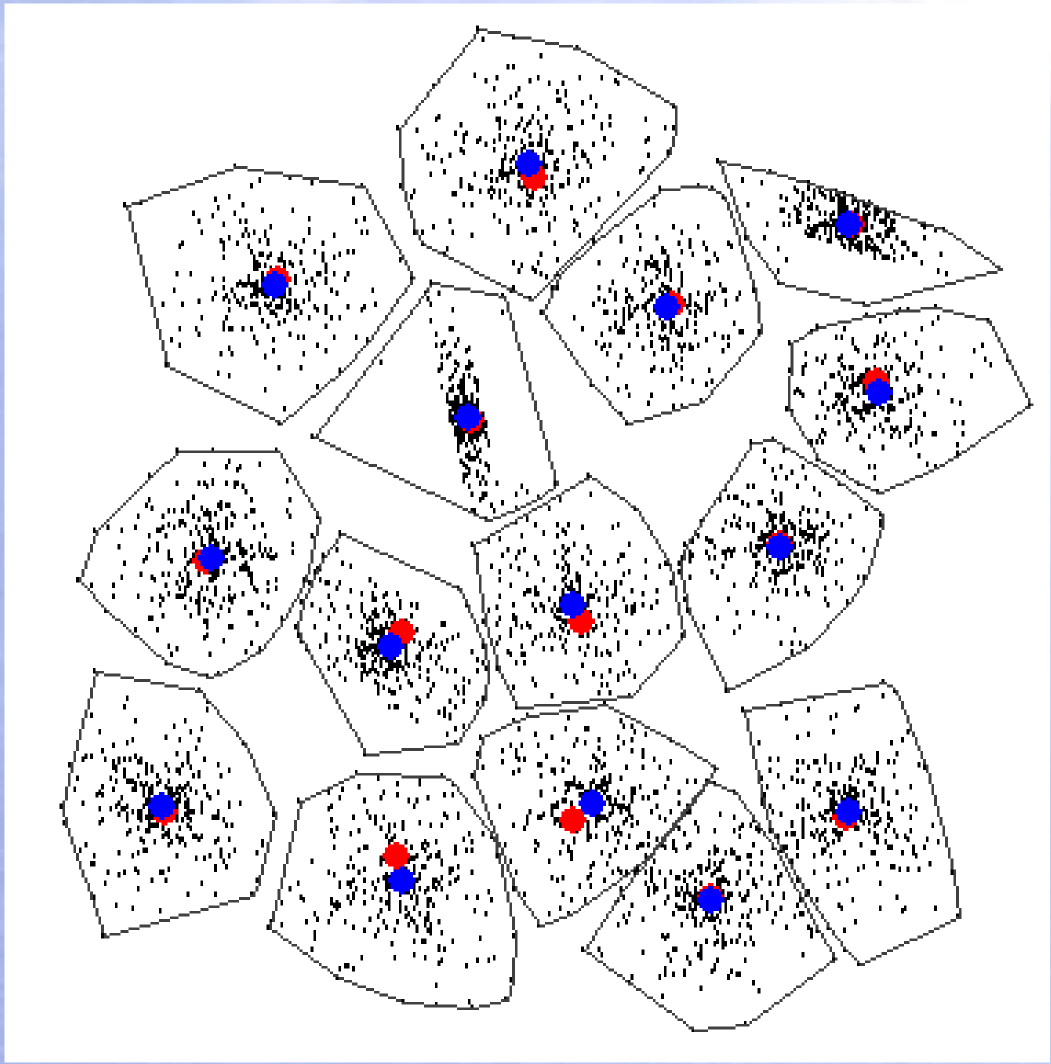
MSE = 1.94

K-means refinement

Result directly after split:
MSE = 1.94

Result after re-partition:
MSE = 1.39

Result after K-means:
MSE = 1.33



Time complexity

Number of processed vectors, assuming that clusters are always split into two equal halves:

$$\sum n_i = N + \left(\frac{N}{2} + \frac{N}{2}\right) + \left(\frac{N}{4} + \frac{N}{4} + \frac{N}{4} + \frac{N}{4}\right) + \ldots + \left(\frac{N}{M/2} + \ldots + \frac{N}{M/2}\right)$$

$$= N + 2 \cdot \frac{N}{2} + 4 \cdot \frac{N}{4} + \ldots \frac{M}{2} \cdot \frac{N}{M/2} = \mathrm{O}(N \cdot \log M)$$

Assuming unequal split to $n_{\max}$ and $n_{\min}$ sizes:

$$n_{\min} \geq p \cdot n_{\max}$$

$$N = n_1 + n_2 + \ldots + n_m \geq m \cdot n_{\min} \geq m \cdot p \cdot n_{\max}$$

$$\Leftrightarrow n_{\max} \leq \frac{N}{p \cdot m}$$

Time complexity

Number of vectors processed:

$$\sum n_i \le \frac{N}{p} + \frac{N}{p \cdot 2} + \frac{N}{p \cdot 3} + \ldots + \frac{N}{p \cdot M}$$

$$= \sum_{m=1}^{M} \frac{N}{p \cdot m} = \mathrm{O}\left(N \cdot \log M\right)$$

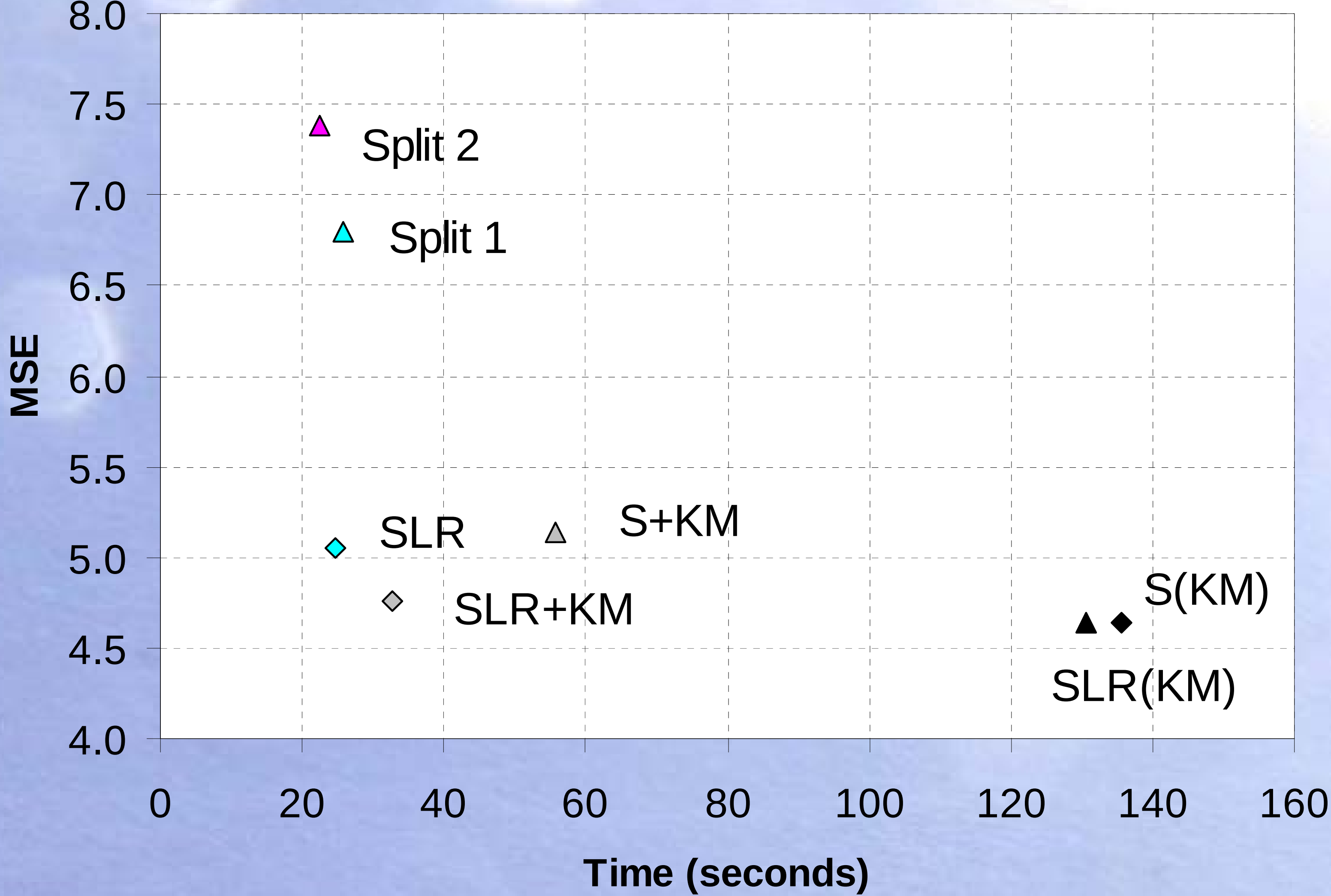
At each step, sorting the vectors is bottleneck:

$$T\left(N\right) = \sum n_i \log n_i \le \sum_{m=1}^{M} \frac{N}{p \cdot m} \log \frac{N}{p \cdot m}$$

$$\le \log \frac{N}{p} \cdot \sum_{m=1}^{M} \frac{N}{p \cdot m} = \mathrm{O}\left(N \cdot \log N \cdot \log M\right)$$

Comparison of results

$Birch_1$



Conclusions

- Divisive algorithms are efficient
- Good quality clustering
- Several non-trivial design choices
- Selection of dividing axis can be improved!

References

1. P Fränti, T Kaukoranta and O Nevalainen, "On the splitting method for vector quantization codebook generation", *Optical Engineering*, 36 (11), 3043-3051, November 1997.
2. C-R Lin and M-S Chen, " Combining partitional and hierarchical algorithms for robust and efficient data clustering with cohesion self-merging", TKDE, 17(2), 2005.
3. M Liu, X Jiang, AC Kot, "A multi-prototype clustering algorithm", *Pattern Recognition*, 42(2009) 689-698.
4. J Shi and J Malik, "Normalized cuts and image segmentation", TPAMI, 22(8), 2000.
5. L Feng, M-H Qiu, Y-X Wang, Q-L Xiang, Y-F Yang, K Liu, "A fast divisive clustering algorithm using an improved discrete particle swarm optimizer", *Pattern Recognition Letters*, 2010.
6. C Zhong, D Miao, R Wang, X Zhou, "DIVFRP: An automatic divisive hierarchical clustering method based on the furthest reference points", *Pattern Recognition Letters*, 29 (2008) 2067–2077.